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THE ROBERT A. WELCH FOUNDATION
62ND CONFERENCE ON CHEMICAL RESEARCH

“WATER: SCIENCE AND TECHNOLOGY”

Monday, October 22, 2018

8:30 **CARIN MARCY BARTH**, Chair of the Board of Directors
8:35 **JAMES L. SKINNER**, University of Chicago, Program Chair

SESSION I – WATER CLUSTERS AND INTERFACES

8:40 **FRANZ M. GEIGER**, Northwestern University, *Discussion Leader*
8:50 **MARK A. JOHNSON**, Yale University
“Tracking the Spectroscopic Behavior of Water Down to the Molecular Level with Temperature Controlled, Size-Selected Clusters”
9:30 Discussion
9:40 **GERALDINE L. RICHMOND**, University of Oregon
“Mulling Over Nanoemulsions: Interfacial Molecular Structure, Stabilization and Assembly”
10:20 Discussion
10:30 Break
10:45 **JAMES T. HYNES**, University of Colorado at Boulder and École Normale Supérieure
“Water Jump Dynamics at Aqueous Interfaces”
11:25 Discussion
11:35 LUNCH

SESSION II – DYNAMICS AND SPECTROSCOPY IN WATER

1:00 **NANCY E. LEVINGER**, Colorado State University, *Discussion Leader*
1:10 **GIULIA GALLI**, University of Chicago
“A Computational Microscope for Water at Interfaces”
1:50 Discussion
2:00 **MICHAEL D. FAYER**, Stanford University
“Water Dynamics Investigated with 2D IR Spectroscopy: Probe Molecules, Salt Solutions, Hydronium Ions, and the Air/Water Interface”
2:40 Discussion
2:50 Break
3:05 **PETER J. ROSSKY**, Rice University
“Understanding Aqueous Clusters, Inside and Out”
3:45 Discussion
3:55 Adjourn

PROGRAM

“WATER: SCIENCE AND TECHNOLOGY”

Tuesday, October 23, 2018

SESSION III – METASTABLE WATER

- 8:00 **BARBARA WYSLOUZIL**, Ohio State University, *Discussion Leader*
- 8:10 **PABLO G. DEBENEDETTI**, Princeton University
“Computational Studies of Supercooled Water”
- 8:50 Discussion
- 9:00 **ANDERS R. NILSSON**, Stockholm University
“X-ray Laser Studies of Supercooled Water”
- 9:40 Discussion
- 9:50 Break
- 10:05 **VALERIA MOLINERO**, The University of Utah
“Crystallization of Water: A Molecular Perspective”
- 10:45 Discussion

2018 Welch Awardee Lecture

- 10:55 **ADRIAAN BAX**, National Institutes of Health
“Protein Structure and Dynamics Derived from Whispering Nuclear Spins”
- 11:35 LUNCH

SESSION IV – WATER TECHNOLOGY

- 1:00 **J. R. SCHMIDT**, University of Wisconsin-Madison, *Discussion Leader*
- 1:10 **DANIEL G. NOCERA**, Harvard University
“Food and Fuel from Sunlight, Air and (Any!) Water”
- 1:50 Discussion
- 2:00 **JUNHONG CHEN**, University of Wisconsin-Milwaukee
“Molecular Engineering of Real-Time Water Sensors Based on 2D Nanomaterials to Enable Intelligent Water Systems”
- 2:40 Discussion
- 2:50 Break
- 3:05 **BENNY D. FREEMAN**, The University of Texas at Austin
“Ion Transport in Charged Polymer Membranes for Water/Energy Applications”
- 3:45 Discussion
- 3:55 Adjourn

**THE ROBERT A. WELCH FOUNDATION
CONFERENCES ON CHEMICAL RESEARCH
1957 – 2018**

<u>YEAR</u>	<u>PRESIDING CHAIR</u>	<u>CONF. NO.</u>	<u>CONFERENCE TITLE</u>
1957	P. J. W. Debye	1	The Structure of the Nucleus
1958	P. J. W. Debye	2	Atomic Structure
1959	Henry Eyring	3	Molecular Structure
1960	Roger Adams	4	Molecular Structure and Organic Reactions
1961	C. Glen King	5	Molecular Structure and Biochemical Reactions
1962	Glenn T. Seaborg	6	Topics in Modern Inorganic Chemistry
1963	Henry Eyring	7	Modern Developments in Analytical Chemistry
1964	Wendell M. Stanley	8	Selected Topics in Modern Biochemistry
1965	Arthur C. Cope	9	Organometallic Compounds
1966	P. J. W. Debye	10	Polymers
1967	Henry Eyring	11	Radiation and the Structure of Matter
1968	Roger Adams	12	Organic Synthesis
1969	Glenn T. Seaborg	13	The Transuranium Elements – The Mendeleev Centennial
1970	W. O. Baker	14	Solid State Chemistry
1971	E. J. Corey	15	Bio-Organic Chemistry and Mechanisms
1972	Henry Eyring	16	Theoretical Chemistry
1973	C. S. Marvel	17	Organic-Inorganic Reagents in Synthetic Chemistry
1974	George W. Beadle	18	Immunochemistry
1975	W. O. Baker	19	Photon Chemistry
1976	Glenn T. Seaborg	20	American Chemistry – Bicentennial
1977	Glenn T. Seaborg	21	Cosmochemistry
1978	Henry Eyring	22	Chemistry of Future Energy Resources
1979	W. O. Baker	23	Modern Structural Methods
1980	Henry Eyring	24	The Synthesis, Structure and Function of Biochemical Molecules
1981	W. O. Milligan	25	Heterogeneous Catalysis
1982	C. S. Marvel	26	Synthetic Polymers
1983	E. J. Corey	27	Stereospecificity in Chemistry and Biochemistry
1984	William N. Lipscomb, Jr.	28	Chemistry in Texas: The 30 th Year of The Welch Foundation
1985	Paul Berg	29	Genetic Chemistry: The Molecular Basis of Heredity
1986	Norman Hackerman	30	Advances in Electrochemistry

<u>YEAR</u>	<u>PRESIDING CHAIR</u>	<u>CONF. NO.</u>	<u>CONFERENCE TITLE</u>
1987	Emil T. Kaiser	31	Design of Enzymes and Enzyme Models
1988	W. O. Baker	32	Valency
1989	Joseph Goldstein	33	Membrane Proteins: Targeting and Transduction
1990	Glenn T. Seaborg	34	Fifty Years with Transuranium Elements
1991	E. J. Corey	35	Chemistry at the Frontiers of Medicine
1992	William N. Lipscomb, Jr.	36	Regulation of Proteins by Ligands
1993	Peter B. Dervan	37	40 Years of the DNA Double Helix
1994	Yuan T. Lee	38	Chemical Dynamics of Transient Species
1995	W. O. Baker Robert A. Laudise	39	Nanophase Chemistry
1996	Norman Hackerman Richard E. Smalley	40	Chemistry on the Nanometer Scale
1997	Glenn T. Seaborg Darleane C. Hoffman	41	The Transactinide Elements
1998	Joseph L. Goldstein	42	The New Biochemistry: Macromolecular Machines
1999	E. J. Corey	43	Synthetic and Biological Chemistry
2000	William N. Lipscomb, Jr.	44	Macromolecular Structures and Function
2001	Peter B. Dervan	45	Chemistry for the 21 st Century
2002	Yuan T. Lee	46	Advances in Quantum Chemistry
2003	Norman Hackerman	47	Chemistry in Texas: Fifty Years of The Welch Foundation
2004	Marye Anne Fox	48	Chemistry of Self-Organized and Hybrid Materials
2005	Norman Hackerman Allan J. Bard	49	Charge Transfer at Electrodes and Biological Interfaces
2006	Joseph L. Goldstein	50	Exploring the complexity of Signaling Pathways
2007	Ahmed H. Zewail	51	Physical Biology – From Atoms to Cells
2008	William N. Lipscomb, Jr.	52	Biological Macromolecules: From Structure to Function
2009	Peter B. Dervan	53	Advances in Synthetic Chemistry
2010	Yuan T. Lee	54	Green Chemistry and Sustainable Energy
2011	Peter G. Schultz	55	From Molecules to Medicine
2012	Richard R. Schrock	56	Advances in Transition Metal Catalyzed Reactions
2013	Roger D. Kornberg	57	Large Problems in Life Chemistry
2014	Marye Anne Fox	58	Chemical Education
2015	Joseph L. Goldstein	59	Next Generation Medicine
2016	Ahmed H. Zewail	60	Frontiers of Imaging
2017	Peter B. Dervan	61	Advances in Synthetic and Biological Chemistry
2018	James L. Skinner	62	Water: Science and Technology

**WELCH AWARD RECIPIENTS
1972 - 2018**

1972	Karl Folkers	1999	Richard N. Zare
1974	Albert Eschenmoser	2000	Sir Alan R. Battersby A. Ian Scott
1976	Neil Bartlett	2001	Roger D. Kornberg
1978	E. Bright Wilson	2002	Harden M. McConnell
1980	Karl Sune D. Bergstrom	2003	Ronald Breslow
1981	Paul D. Bartlett	2004	Allen J. Bard
1982	Frank H. Westheimer	2005	George M. Whitesides
1983	Henry Taube	2006	Daniel E. Koshland, Jr.
1984	Kenneth S. Pitzer	2007	Noel S. Hush William H. Miller
1985	Duilio Arigoni	2008	Alexander Rich
1986	George C. Pimentel	2009	Harry B. Gray
1987	Harry G. Drickamer	2010	JoAnne Stubbe Christopher T. Walsh
1988	Richard B. Bernstein	2011	John S. Waugh
1989	Norman R. Davidson	2012	David E. Evans
1990	William von Eggerts Doering John D. Roberts	2013	Louis E. Brus
1991	Edwin G. Krebs Earl R. Stadtman	2014	Robert G. Bergman
1992	Richard E. Smalley	2015	Stephen C. Harrison
1993	Gilbert Stork	2016	Richard H. Holm Stephen J. Lippard
1994	F. Albert Cotton Jack Halpern	2017	John B. Goodenough
1995	Robert H. Abeles Jeremy R. Knowles	2018	Adriaan Bax
1996	Koji Nakanishi		
1997	Ahmed H. Zewail		
1998	Pierre Chambon		

HACKERMAN AWARD RECIPIENTS

2002 - 2018

2002	Andrew R. Barron
2003	Xiaodong Wang
2004	Jianpeng Ma
2005	Zhijian J. Chen
2006	Paul S. Cremer
2007	Patrick G. Harran
2008	Francis T. F. Tsai
2009	Cecilia Clementi
2010	Kimberly A. Orth-Taussing
2011	Jason H. Hafner
2012	Oleg V. Ozerov
2013	Olafs Daugulis
2014	Benjamin P. Tu
2015	Stephan Link
2016	Christopher J. Ellison
2017	Neal M. Alto Delia J. Milliron
2018	Jeffrey D. Rimer

PRINCIPAL INVESTIGATORS

2017 - 2018

Abrams	John M.	I-1865	Conrad	Nicholas K.	I-1915
Ahn	Jung-Mo	AT-1595	Contreras	Lydia M.	F-1756
Alto	Neal M.	I-1704	Corey	David R.	I-1244
Alù	Andrea	F-1802	Cuny	Gregory	E-1916
Aronson	Meigan	A-1890	Dai	Pengcheng	C-1839
Bahadur	Vaibhav	F-1867	Dalby	Kevin N.	F-1390
Baiz	Carlos R.	F-1891	Danuser	Gaudenz	I-1840
Balkus, Jr.	Kenneth J.	AT-1153	Darensbourg	Donald J.	A-0923
Ball	Zachary T.	C-1680	Darensbourg	Marcetta Y.	A-0924
Banaszynski	Laura	I-1892	Davies	Bryan W.	F-1870
Bao	Jiming	E-1728	De Brabander	Jef K.	I-1422
Barondeau	David P.	A-1647	Deberardinis	Ralph J.	I-1733
Barrick	Jeffrey E.	F-1780	Deem	Michael W.	C-1917
Bartel	Bonnie	C-1309	Dias	H. V. Rasika	Y-1289
Belkin	Mikahil A.	F-1705	Do	Loi H.	E-1894
Bennett	Matthew R.	C-1729	Dodani	Sheel	AT-1918
Bergbreiter	David E.	A-0639	Doncic	Andreas	I-1919
Bernal	Ricardo A.	AH-1649	D'Orso	Ivan	I-1782
Billups	W. E.	C-0490	Douglas	Peter	I-1920
Bittner	Eric R.	E-1337	Downer	Michael C.	F-1038
Blount	Paul	I-1420	Doyle	Michael P.	AX-1871
Brodbelt	Jennifer S.	F-1155	Du	Rui-Rui	C-1682
Brookhart	Maurice	E-1893	Dunbar	Kim R.	A-1449
Bruick	Richard K.	I-1568	Dunning	F. Barry	C-0734
Burgess	Kevin	A-1121	Elber	Ron	F-1896
Burgess	Shawn C.	I-1804	Ellington	Andrew D.	F-1654
Chapman	Walter G.	C-1241	Erzberger	Jan P.	I-1897
Chelikowsky	James R.	F-1837	Fan	Donglei L.	F-1734
Chen	Banglin	AX-1730	Fang	Lei	A-1898
Chen	Chuo	I-1868	Fast	Walter L.	F-1572
Chen	Zheng	AU-1731	Fatehi	Shervin	BX-1921
Chen	Zhijian J.	I-1389	Findlater	Michael	D-1807
Chiang	Cheng-Ming	I-1805	Finkelstein	Ilya J.	F-1808
Chook	Yuh Min	I-1532	Fitzpatrick	Paul F.	A-1245
Chuang	David T.	I-1286	Fortier	Skye	AH-1922
Clearfield	Abraham	A-0673	Foster	Matthew S.	C-1809
Clementi	Cecilia	C-1570	Frederick	Kendra K.	I-1923
Cobb	Melanie H.	I-1243	Freeman	Benny D.	F-1924
Coffer	Jeffery L.	P-1212	Gabbaï	François P.	A-1423
Coltart	Don M.	E-1806	Gallagher	Elyssia S.	AA-1899
Conacci-Sorrell	Maralice	I-1914	Ganesan	Venkat	F-1599
Conrad	Jacinta C.	E-1869	Garcia-Bosch	Isaac	N-1900

**PRINCIPAL INVESTIGATORS
2017 - 2018**

Gladysz	John A.	A-1656	Jones	Richard A.	F-0816
Gohil	Vishal M.	A-1810	Jose Yacaman	Miguel	AX-1615
Golding	Ido	Q-1759	Kadish	Karl M.	E-0680
Goldsmith	Elizabeth J.	I-1128	Kaplan	Craig D.	A-1763
Goodenough	John B.	F-1066	Keatinge-Clay	Adrian T.	F-1712
Grigolini	Paolo	B-1577	Keitz	Ben	F-1929
Grishin	Nick V.	I-1505	Kiang	Ching-Hwa	C-1632
Guloy	Arnold M.	E-1297	Killian	Thomas C.	C-1844
Hafner	Jason H.	C-1761	Kim	Nayun	AU-1875
Halas	Naomi J.	C-1220	Kirienko	Natasha	C-1930
Halasyamani	P. Shiv	E-1457	Kliwer	Steven A.	I-1558
Hall	Michael B.	A-0648	Ko	Che Ming	A-1358
Hardy	John C.	A-1397	Kohler	Jennifer J.	I-1686
Harshey	Raskia M.	F-1811	Kolomeisky	Anatoly B.	C-1559
Hart	P. John	AQ-1399	Kono	Junichiro	C-1509
Hartgerink	Jeffrey D.	C-1557	Korgel	Brian A.	F-1464
Hazzard	Kaden	C-1872	Kürti	László	I-1764
Heller	Adam	F-1131	Laane	Jaane	A-0396
Henkelman	Graeme	F-1841	Lai	Keji	F-1814
Henne	W. Mike	I-1873	Lambowitz	Alan M.	F-1607
Hibbs	Ryan E.	I-1812	Landes	Christy F.	C-1787
Hildebrandt Ruiz	Lea	F-1925	Larionov	Oleg V.	AX-1788
Hilty	Christian B.	A-1658	Latham	Michael	D-1876
Hoffman	David M.	E-1206	Lee	Seongmin	F-1741
Hon	Gary Chung	I-1926	Lee	T. Randall	E-1320
Hooper	Lora V.	I-1874	Li	Guigen	D-1361
Hsu	Julia W.P.	AT-1843	Li	Pingwei	A-1931
Hulet	Randall G.	C-1133	Li	Wei	C-1845
Humphery	Simon M.	F-1738	Li	Wen-hong	I-1902
Hwang	Gyeong S.	F-1535	Li	Xiaoqin (Elaine)	F-1662
Igumenova	Tatyana I.	A-1784	Lieberman Aiden	Erez	Q1866
Iverson	Brent L.	F-1188	Lindahl	Paul A.	A-1170
Jaqaman	Khuloud	I-1901	Link	Stephan	C-1664
Jayaram	Makkuni	F-1274	Liou	Jen	I-1789
Jewell	Jenna	I-1927	Liu	Hung-wen	F-1511
Jiang	Jean X.	AQ-1507	Liu	Jun	AU-1714
Jiang	Jin	I-1603	Liu	Qinghau	I-1608
Jiang	Ning	F-1785	Liu	Wenshe	A-1715
Jiang	Youxing	I-1578	Liu	Xin	I-1790
Joachimik	Lukasz A.	I-1928	Liu	Yi	I-1560
Johnson	Kenneth A.	F-1604	Lockless	Steve W.	A-1742
Johnston	Keith P.	F-1319	Lou	Jun	C-1716

PRINCIPAL INVESTIGATORS

2017 - 2018

Lovely	Carl J.	Y-1362	Orth	Kim	I-1561
Lubchenko	Vassiliy	E-1765	Ozerov	Oleg V.	A-1717
Lucchese	Robert R.	A-1020	Palmer	Jeremy C.	E-1882
Lum	Lawrence	I-1665	Pannell	Keith H.	AH-0546
Lumata	Lloyd L.	AT-1877	Pasquali	Matteo	C-1668
Luo	Weibo	I-1903	Phillips	Margaret A.	I-1257
Lou	Xuelian	I-1932	Poirier	Lionel W.	D-1523
Lynd	Nathaniel A.	F-1904	Powers	David C.	A-1907
Ma	Jianpeng	Q-1512	Prasad	B. V. Venkataram	Q-1279
MacDonald	Allan H.	F-1473	Pu	Han	C-1669
MacDonnell	Frederick M.	Y-1933	Que	Emily L.	F-1883
Maeder	Corina	W-1905	Radhakrishnan	Arun	I-1793
Makarov	Dmitrii E.	F-1514	Raizen	Mark G.	F-1258
Mangelsdorf	David J.	I-1275	Ranganathan	Raman	I-1366
Manthiram	Arumugam	F-1254	Raushel	Frank M.	A-0840
Marcotte	Edward M.	F-1515	Ready	Joseph M.	I-1612
Martin	Caleb D.	AA-1846	Reese	Michael	I-1936
Martin	Stephen F.	F-0652	Reichl	Linda E.	F-1051
Martinez	Elisabeth D.	I-1878	Ren	Pengyu	F-1691
Matouschek	Andreas	F-1817	Rentzepis	Peter M.	A-1884
May	Jeremy A.	E-1744	Rice	Luke M.	I-1908
Maynard	Jennifer A.	F-1767	Richmond	Michael G.	B-1093
Meeks	Julian	I-1934	Rimer	Jeffrey D.	E-1794
Meloni	Gabriele	AT-1935	Rizo-Rey	Jose	I-1304
Miljanić	Ognjen Š.	E-1768	Roberts	Sean T.	F-1885
Milliron	Delia J.	F-1848	Romo	Daniel	A-1280
Mukhopadhyay	Saikat	I-1906	Rose	Michael J.	F-1822
Mullins	Charles B.	F-1436	Rosen	Michael K.	I-1544
Nam	Yunsun	I-1851	Rosenbaum	Daniel M.	I-1770
Natelson	Douglas	C-1636	Ross, Jr.	Joseph H.	A-1526
Naugle	Donald G.	A-0514	Rossky	Peter	C-1937
Nevidomskyy	Andriy	C-1818	Russell	Rick	F-1563
Nicolaou	Kyriacos C.	C-1819	Schiavinato Eberlin	Livia	F-1895
Nijhawan	Deepak	I-1879	Schmid	Sandra L.	I-1823
Nippe	Michael	A-1880	Schuessler	Hans A.	A-1546
Niu	Qian	F-1255	Scully	Marlan O.	A-1261
Nordlander	Peter J.A.	C-1222	Sczepanski	Jonathan T.	A-1909
North	Simon W.	A-1405	Seemann	Joachim	I-1910
O'Donnell	Kathryn A.	I-1881	Segatori	Laura	C-1824
Olson	John S.	C-0612	Shan	Libo	A-1795
Omary	Mohammad A.	B-1542	Shaw	Bryan F.	AA-1854
Onuchic	José	C-1792			

PRINCIPAL INVESTIGATORS
2017 - 2018

Shear	Jason B.	F-1331	Willson	C. Grant	F-1830
Sheldon	Matthew	A-1886	Wilson	Lon J.	C-0627
Sherry	A. Dean	AT-0584	Wu	Jiang	I-1940
Shi	Xioabing	G-1719	Xie	Chong	F-1941
Shih	Chih-Kang	F-1672	Xu	Jian	I-1642
Si	Qimiao	C-1411	Yakobson	Boris I.	C-1590
Siegwart	Daniel J.	I-1855	Yan	Nan	I-1831
Sokolov	Alexei V.	A-1547	Yang	Ding-Shyue	E-1860
Son	Dong Hee	A-1639	Ye	Jin	I-1832
Songyang	Zhou	Q-1673	Yeager	Danny L.	A-0770
Stefan	Mihaela C.	AT-1740	Yeh	Hsin-Chih	F-1833
Su	Wu-Pei	E-1070	Yennello	Sherry J.	A-1266
Tabor	Jeffrey J.	C-1856	Yu	Guihua	F-1861
Tagiabracci	Vincent S.	I-1911	Yu	Hongtao	I-1441
Tambar	Uttam K.	I-1748	Yu	Yonghao	I-1800
Tao	Yizhi Jane	C-1565	Zakhidov	Anvar A.	AT-1617
Taylor	David	F-1938	Zhang	Chengcheng	I-1834
Teets	Thomas S.	E-1887	Zhang	Chun-Li	I-1724
Terman	Jonathan R.	I-1749	Zhang	Junjie	A-1863
Thummel	Randolph P.	E-0621	Zhang	Renyi	A-1417
Ting	Chin-Sen	E-1146	Zhang	Xuewu	I-1702
Tittel	Frank K.	C-0586	Zhang	Yan Jessie	F-1778
Tonzetich	Zachary J.	AX-1772	Zhao	John C.-G.	AX-1593
Truskett	Thomas M.	F-1696	Zheltikov	Alexey M.	A-1801
Tsai	Francis T.F.	Q-1530	Zhong	Qing	I-1684
Tu	Benjamin P.	I-1797	Zhu	Yubin	BE-1913
Urbach	Adam R.	W-1640			
Uyeda	Kosaku	I-1720			
Verduzco	Rafael	C-1888			
Wagner	Eric J.	H-1889			
Wan	Yihong	I-1751			
Wang	Meng C.	Q-1912			
Wang	Qinghua	Q-1826			
Wang	Yingfei	I-1939			
Wang	Yuhong	E-1721			
Wang	Zhigao	I-1827			
Watanabe	Coran	A-1828			
Webb	Lauren J.	F-1722			
Weisman	R. Bruce	C-0807			
Westover	Kenneth D.	I-1829			
Whetten	Robert L.	AX-1857			
Whitman	Christian P.	F-1334			

ABSTRACTS OF CURRENT INVESTIGATIONS*

The following Abstracts, as supplied by the Principal Investigators in the Research Grant Program, Endowed Chair Program, Miscellaneous Grants, and Other Endowments, describe some of the current research work in chemistry being supported by the Foundation.

*The abstracts recorded in this annual report supplement are published exactly as they were submitted.

JOHN M. ABRAMS, I-1865, The University of Texas Southwestern Medical Center. APOPTOSOME CASPASE CONTROL BY Tango7.

The working model developed under this grant probes Tango7 as a regulatory adaptor that couples specific substrates to the apoptosome, thereby instructing proteolytic activities that arbitrate distinct cell fates. We searched for substrates that are selectively targeted by remodeling apoptosomes but not cleaved by apoptogenic apoptosomes. From these screens, we discovered Glutamine: fructose -6-phosphate aminotransferase (GFAT) as a high priority candidate. Importantly, we established that cleavage of this substrate occurred only in cells that were remodeling but not cells that were dying. These in vivo results demonstrate that distinct substrate profiles are indeed coupled to distinct cell fates. To our knowledge, this is the first identification of a substrate that is cleaved when apoptosomes remodel cells but is not cleaved when this same complex is killing cells. The genome encodes two GFAT enzymes (GFAT 1 and GFAT2) and, using complementary strategies, we are determining which of these proteins is the authentic, in vivo substrate. Toward this end, we combined Gibson Assembly methods and CRISPR-CAS9 technologies to produce single-lesion mutations in both of these genes. We are in the process of characterizing these mutants and both are embryonic lethal. Interestingly, and consistent with distinct functions for these genes, treatment with the enzymatic product (D - Glucosamine 6- Phosphate) can be used to rescue GFAT2 mutants but the same treatment does not rescue GFAT1 mutants. Studies in progress are leveraging these and related tools to understand the biochemistry that explains caspase-dependent remodeling.

JUNG-MO AHN, AT-1595, The University of Texas at Dallas. TAILORING SMALL MOLECULES TO MIMIC PROTEIN HELICAL SURFACES.

In the first grant year, we have started the synthesis of a small molecular library (64 members in total) based on the extended biphenyl scaffold. To the end, we have synthesized two sets of 8 bis-benzamides, one with an iodide and the other with a boronic acid, which were coupled together via Suzuki-Miyaura cross-coupling in the presence of Pd catalyst. We found the coupling reaction generally proceeded well with a high yield, but some failed presumably because of steric hindrance resulting from the structures of two components. For such a case, we have surveyed bases, reaction temperatures, and different Pd catalysts, and managed to obtain an improved yield. To date, we have prepared 28 biphenyl compounds that carry 4 diverse side chain functional groups. They have been first examined on their binding affinity to Bcl-xL and Bcl-2 proteins by using fluorescence polarization assays and then their cytotoxicity on prostate cancer cell lines like DU145, PC3, and LNCaP. We found some of them showed strong binding affinity to Bcl-xL and Bcl-2 (e.g., 1-2 μ M as their IC50 values). We are currently trying to establish experimental conditions to carry out protein binding assays with Mcl-1. Using a GST-Mcl-1 plasmid, we have attempted to express the Mcl-1 protein in BL21 and isolate it by GST tag affinity column. While we have encountered an inclusion body problem during the expression in BL21, we managed to get the functional protein expressed by lowering the incubation temperature during expression process. In the meantime, we have carried out the synthesis of the new spiro-piperidine scaffold. We have done nucleophilic aromatic substitution reactions to make various arylpiperidinone and made the spiro ring structure with several diamines. We have encountered some problems in this reaction and are currently trying to address the issues by modifying experimental conditions, functional groups, and structures of starting materials.

NEAL M. ALTO, I-1704, The University of Texas Southwestern Medical Center. POST-TRANSLATIONAL MODIFICATION OF HOST ENZYMES BY BACTERIAL EFFECTOR PROTEINS.

We completed the major goals of the past grant application, which was to define the molecular mechanisms of two homologous *Shigella flexneri* Type III Secretion System (T3SS) effector E3 ligases IpaH1.4 and IpaH2.5. Given the success of this project, we are now pursuing a new avenue in host-pathogen interactions. There have been very few bacterial E3-ubiquitin ligase substrates identified and the reaction mechanism of microbial-based ubiquitylation remains poorly understood. We successfully developed a bacterial E3-ligase screening methodology that relies on the formation of a covalent enzyme- substrate complex and identification by mass spectrometry. This work has revealed that the orphan E3-ubiquitin ligase IpaH7.8 directly ubiquitinates members of the Gasdermin family. Gasdermins belong to a newly discovered family of eukaryotic pore-forming cytolysins. The founding member of this family, Gasdermin-D, functions as the primary executioner of the inflammatory cell death program known as pyroptosis. Because this is a completely new direction for my laboratory, we are now pursuing the biochemical and structural nature of this host-pathogen interaction through biochemistry and X-ray crystallography. In addition, we are developing a transgenic mouse model of Gasdermin-B function as a platform for translating biochemical studies into the broader context of bacterial infectious disease.

Importantly, understanding how bacterial pathogens regulate pyroptotic cell death through destruction of Gasdermin family members will address fundamental questions in enzyme chemistry, human signaling and bacterial pathogenesis, and could lead to practical development of drugs aimed at curing microbial infectious disease. Lastly, our work on the biochemistry of bacterial effector proteins has garnered significant support including the first Presidential Scholar Award from UTSW.

ANDREA ALÙ, F-1802, The University of Texas at Austin. GIANT SENSITIVITY AND BROADBAND CIRCULAR DICHROISM IN PLASMONIC METAMATERIALS.

In the second year of this effort, we have done exciting progress in advancing optical metasurfaces for chemistry related applications, most specifically bio-sensing and optical wave manipulation. First, we have significantly advanced the field of gradient metasurfaces, by introducing the concept of meta-gratings and their practical implementation. This is an important result, since metasurfaces to date have been inherently inefficient, and they are our proposed platform for wave manipulation and biomedical / chemical detection. We have been applying these advances for light management, focusing, polarization control, wavefront shaping with large efficiency, and to enhance molecular emission and light-matter interactions. As a second important thrust of our activity in this project, we have made substantial progress on the concept of bound states in the continuum and embedded eigenstates, proving their

potential impact for chemical sensing, and experimentally verifying their inherent topological signature in the far-field. Our results have appeared in several peer-reviewed publications, including high-profile papers in Physical Review and Nature journals. We are excited to continue this work, and steer it to the application for chemical sensing in the final year of this project.

MEIGAN ARONSON, A-1890, Texas A&M University. ACCELERATING THE SEARCH FOR NEW TOPOLOGICAL MATERIALS USING IN-SITU X-RAY DIFFRACTION MEASUREMENTS AND ELECTRONIC STRUCTURE CALCULATION.

We used in situ xray diffraction experiments, carried out on beamline 6-ID-D at Argonne National Lab, to establish the phase diagram La_2CuO_4 - $\text{La}_2\text{Cu}_3\text{S}_4$. Attempts to synthesize the ordered compound $\text{La}_2\text{CuO}_3\text{S}$ from $\text{La}_2\text{O}_2\text{S}$ and CuO resulted in the formation of LaCuSO plus La_2O_3 , via a two step reaction: $\text{La}_2\text{O}_2\text{S}$ and CuO first react at ~ 760 C, forming $\text{La}_2\text{O}_2\text{SO}_4$ and Cu_2O . At higher temperature, the newly formed Cu_2O reacts with the remaining $\text{La}_2\text{O}_2\text{S}$, forming LaCuSO and La_2O_3 . The energies of these two experimental reactions have also been computed. Both steps have negative reaction energies, indicating these are thermodynamically favorable reactions. Reaction step 1 where $\text{La}_2\text{O}_2\text{S} + 8 \text{CuO} = 4 \text{Cu}_2\text{O} + \text{La}_2\text{O}_2\text{SO}_4$ has an especially negative energy 197 meV/atom, which provides a large thermodynamic driving force for the forward reaction, compared to the proposed reaction $\text{La}_2\text{O}_2\text{S} + \text{CuO} = \text{La}_2\text{CuO}_3\text{S}$, which has instead a large positive energy 182 meV/atom. This research was recently published in the Proceedings of the National Academy of Sciences (<https://doi.org/10.1073/pnas.1800284115>).

More recently, we have used in situ XRD in a project to synthesize single crystals of the newly discovered Dirac semimetal Ca_3P_2 from flux. In the course of several hours, we were able to test 5 different possible fluxes: NaCl , KCl , In , Bi , and Sn . Only in KCl , In , and Sn was it possible to dissolve the reactants to form a homogeneous melt, and only in KCl was it further possible to avoid forming compounds other than Ca_3P_2 on cooling the melt. Following this prescription, we were able to form small single crystals of Ca_3P_2 , which were found by XRD to be P-deficient. In order to place the Dirac point at the Fermi level, hole doping would be required. This work continues.

VAIBHAV BAHADUR, F-1867, The University of Texas at Austin. ROLE OF SURFACE CHEMISTRY AND INTERFACIAL CHARGE ON METHANE HYDRATE NUCLEATION.

Two experimental setups were fabricated and used to study electronucleation of THF hydrates:

Setup for measurements of electronucleation.

Setup to study influence of electrode material and metal foams on electronucleation. The development of two experimental setups is ongoing. These include:

A high pressure, 450 ml reactor to study methane hydrate nucleation.

A setup to study nucleation of cyclopentane hydrates.

The following fundamental studies were completed:

Review of physical/chemical mechanisms underlying electrofreezing (1 journal article published)

This article reviewed the fundamental mechanisms underlying electrofreezing of ice. Studies from 1851 onwards were analyzed. Topics reviewed include experimental studies of electrofreezing, pyroelectricity- based control of freezing and molecular dynamics simulations.

Influence of electrode material and electrochemistry on electronucleation (1 journal article being prepared)

Previous research uncovered two distinct interfacial mechanisms underlying electronucleation, namely electrolytic bubble generation, and the formation of metal ion complexes in solution. Research in the past year further uncovered the role of electrochemistry on nucleation. Experiments were conducted with variable electrode materials, including aluminum, copper and carbon. Aluminum electrodes enhanced nucleation, with electrode polarity playing a key role. On the other hand, the nucleation enhancement due to copper electrodes was polarity-independent. Copper promotes faster electronucleation as compared to other electrode materials.

Influence of metal foams on electronucleation (1 journal article being prepared)

Metal foams as electrodes assist nucleation by providing active nucleation sites. Additionally, the foam material plays a significant role. This study compared foam-based electronucleation of THF hydrates with copper, aluminum and carbon as three metals characterized.

CARLOS R. BAIZ, F-1891, The University of Texas at Austin. STUDIES IN BIOPHYSICAL CHEMISTRY: APPLICATIONS OF ULTRAFAST INFRARED SPECTROSCOPY.

We have successfully completed the first phase of this project which involved characterizing the structure of peptides in a lipid membrane, under equilibrium conditions. We have submitted a manuscript to Biophysical Journal where we report the interfacial dynamics of a lipid bilayer using experiments and simulations, in collaboration with Prof. Ron Elber (F-1896). This manuscript describes the effect of calcium ions, at physiological concentrations, on the dynamics at the lipid/water interface. The manuscript is currently under review. Our second manuscript on the project is complete and ready for submission to Biochemistry (ACS journal). This manuscript quantifies the degree of water penetration into a lipid membranes using a peptide as the "probe" of its immediate hydration environment.

We have recently purchased a UV laser to begin the second phase of the project. The carry-forward from the previous period is due to the budget for the laser (\$16,210), along with the required optics (\sim \$4,000) and electronics (\sim 2,000), which was projected to be spent during this period. We recently received the laser, and we began integrating the new laser within our 2D IR setup. We estimate the the building phase and preliminary experiments will require 3-4 months, and we should be able to carry out the proposed experiments within the 2018-19 period.

KENNETH J. BALKUS, JR., AT-1153, The University of Texas at Dallas. ZEOLITE ENCAPSULATED METAL COMPLEXES.

We have made significant progress during the most recent funding period on the synthesis and modification of zeolitic materials which includes metal organic frameworks (MOF) and carbons. We have continued to work with the wrinkled silica and found that hollow spheres can be made which encapsulate guest molecules during synthesis. We are currently following up on the range of nanoparticles and applications of these host guest materials. Previously we had reported using wrinkled mesoporous silica as a template to make nanocast carbons that were shown to be excellent catalyst supports and selective adsorbents. In particular, the carbons have a high affinity for rare earth and certain actinide elements. Lanthanum oxides supported on silica or as free standing nanoparticles were found to be effective catalysts for carbon formation via an acetylide complex. This work has been extended to related yttrium nanoparticles and calcium oxide. Several new metal organic frameworks have been prepared, including more than a dozen new structures that incorporate Holmium as a node. Holmium is of interest because of the potential applications in radiation therapy and gas separations.

ZACHARY T. BALL, C-1680, Rice University. NEW STRATEGIES FOR CATALYTIC BOND FORMATION.

Scientific efforts continue to focus on reaction discovery with biological substrates, new paradigms for reaction selectivity in complex environments, and the application of these discoveries to protein chemistry, chemical biology, and human health. We have recently explored the concept of “a single protein as combinatorial library”: Can the broad chemical and structural diversity of a single protein be harnessed to discover interesting new reactivity? Screening whole protein substrates has indeed allowed the discovery of four new and unknown reactions for protein modification (three published, one under review), each targeting different protein sites/residues, mediated by Ni²⁺, Cu²⁺, Rh³⁺, and the organic redox-mediator ascorbate. Perhaps most importantly we have developed important new directions for our copper-catalyzed backbone N-H arylation/alkenylation reaction directed by histidine residues. First, we designed a vinylboronic acid reagent that allows formation of a photocleavable backbone modification (pub 61).

This capability allows photocaging backbone structure, and thus photocontrol of folding and function. It also represents a rare example of photocleavage at an C(sp²) alkenyl site.

The uncommon amino acid pyroglutamate, encoded in natural proteins by the enzyme glutaminyl cyclase (QC), has become an important area of study. Pyroglutamate-histidine sequences have unique and profound reactivity in Cu- and Ni-catalyzed processes. This reactivity has allowed us to develop a minimalist, readily-encoded reactive tag, and ongoing studies in the lab have uncovered other new reactivity of this unique and underappreciated residue.

Medicinal chemistry efforts continue in the areas of antibody-drug conjugates and of the STAT3 pathway as an anti-leukemia target. Animal studies with STAT3 inhibitors developed in our lab have shown significant promise, and synergistic activity with known anti-leukemia agents points to a novel mechanism of action for the STAT3 pathway.

LAURA BANASZYNSKI, I-1892, The University of Texas Southwestern Medical Center. ROLE OF CHROMATIN REMODELING IN ALTERNATIVE POSITIVE CANCERS.

Our recent studies and others have shown that the ATRX/DAXX complex is recruited to heterochromatic GC-rich regions such as telomeres, and that loss of ATRX is associated with loss of heterochromatin and increased transcription from these regions. Additional studies have suggested that ATRX may mediate replication through heterochromatic regions by facilitating fork progression through non-B form DNA structures common to heterochromatin. However, mechanisms recruiting the ATRX/DAXX complex to these regions remain unknown. The goal of our research is to identify mechanisms involved in recruitment of ATRX/DAXX to heterochromatic regions to better understand how their loss results in tumor progression.

Previously, we used mass spectrometry to identify a novel interaction between ATRX and the MCM2/4/6 DNA helicase, a critical component of the DNA replication machinery. In the past year, we have validated this interaction and used genomic data sets to generate new hypotheses based on this interaction. Specifically, we have used Proximity Ligation Assay (PLA) to demonstrate nuclear colocalization of ATRX and the MCM proteins. In support, we observe that ATRX KO cells show defects in cell cycle progression and experience replication stress. Our analysis of published data sets shows that ATRX localizes to late-replicating regions of chromatin that are typically heterochromatic and may contain stable secondary structures such as G-quadruplexes and R-loops. Together, these observations support our hypothesis that one of the major functions of ATRX is to promote DNA polymerase passage through regions of DNA containing stable secondary structures. We have generated genome-wide maps of R-loop localization in WT and ATRX KO cells. We are analyzing these data to determine whether R-loop persistence is altered in the absence of ATRX. We are also generating a high-quality data set to determine ATRX enrichment genome-wide that we will correlate with our R-loop data set.

JIMING BAO, E-1728, University of Houston. DISTINGUISHING PHOTOCATALYTIC ACTIVITY OF DIFFERENT COBALT OXIDES THROUGH CONTROLLED MATERIAL SYNTHESIS AND SYSTEMATIC PHOTOELECTROCHEMICAL INVESTIGATION.

- Synthesized Co₃O₄ nanoparticles with size from 3 nm to more than 10 nanometers using a hydrothermal method. Observed a broad band size-dependent photoluminescence of Co₃O₄.
- Synthesized Pt/Co₃O₄ nanoparticles heterostructures and observed water splitting.
- Synthesized phase-pure FeP, Fe₂P and Fe₃P films and systematically investigated their hydrogen evolution activity.
- Demonstrated trimetallic NiFeMo alloy as an efficient overall water splitting catalyst.
- Demonstrated bifunctional metal phosphide FeMnP films as an efficient overall water splitting electrocatalyst.

- Demonstrated vertically aligned MoS₂/Mo₂C hybrid nanosheets for efficient electrocatalytic hydrogen evolution by making use of high electrocatalytic hydrogen evolution reactivity of ultrafine Mo₂C nanocrystals and edges of two-dimensional MoS₂.
- We have demonstrated hierarchical CoP/Ni₅P₄/CoP microsheet arrays as a robust pH-universal electrocatalyst for efficient hydrogen generation; hierarchical Cu@CoFe layered double hydroxide core-shell nanoarchitectures as bifunctional electrocatalysts for efficient overall water splitting; high-performance bifunctional porous non-noble metal phosphide catalyst for overall water splitting.
- We have discovered photoacoustic laser streaming and demonstrated gold implanted quartz window as a launch pad for photoacoustic laser streaming on demand; we have also achieved planar alignment of graphene sheets and observed many of its interesting optical properties; we identified a new luminescent defect state in two-dimensional perovskite-related materials; we observed 1.27 μm photoluminescence from oxygen singlet from graphene dots, and we demonstrated an infrared light-emitting diode based on highly efficient red-emitting bis-cyclometalated iridium complexes.

DAVID P. BARONDEAU, A-1647, Texas A&M University. EVOLVING METALLOCOFACTOR CHEMISTRY THROUGH SECOND SHELL INTERACTIONS.

In the last year, we published an article on the crystal and electron microscopy structure coupled to functional studies of the mitochondrial cysteine desulfurase (NFS1-ISD11-ACP) complex (Proc. Natl. Acad. Sci 2017 Jul 3; 114(27) E5325-5334). The study revealed a novel architecture for a cysteine desulfurase and provide new insight into the role of the mitochondrial acyl carrier protein and the LYRM protein family. We conducted additional mutagenesis coupled to spectroscopic and functional experiments to understand the activity tuning of HydY, a new class of [FeFe]-hydrogenase fusion proteins. This revised manuscript is ready to be submitted. We have also determined the crystal structure of the hydrogen peroxide reductase domain of HydY and will conduct some additional biochemical studies and submit this study for publication. We have used stopped-flow studies to decipher the allosteric function of FXN (manuscript will be resubmitted to PNAS) and CyaY (manuscript under preparation for ACS chemical biology) in Fe-S cluster biosynthesis. We have also completed fluorophore labeling and kinetic analysis studies that suggest dithiol glutaredoxins function in Fe-S cluster storage (prepared for Biochemistry).

JEFFREY E. BARRICK, F-1780, The University of Texas at Austin. COMPARING THE CHEMICAL UTILITY OF ALTERNATIVE GENETIC CODES.

We previously developed a computational framework built around the Rosetta molecular modeling suite for predicting the energetic and functional consequences of nonstandard amino acid (nsAA) substitutions and applied it to TEM-1 beta-lactamase. This year, we further extended this framework, including by creating a point charge model of the amino acid iodotyrosine that can mimic its ability to form halogen bonds. Then, we used this framework to analyze substitutions of nsAAs in bacteriophage T7 RNA polymerase that we observed during the evolution experiment. We predict that the most widespread substitution that which evolved in parallel in different phage populations (tryptophan-88 to iodotyrosine) is positioned such that it can form a halogen bond and adjust the interaction of RNA polymerase with the DNA promoter.

To test the biochemical effects of the iodotyrosine substitution for tryptophan-88, we purified T7 RNA polymerase variants with tryptophan, tyrosine, iodotyrosine and other nonstandard amino acids at position 88. We found that the iodotyrosine variant produced a marked increase in transcriptional output compared to wild-type tryptophan or the tyrosine mutant, most notably at the weaker 'early' promoters of the phage genome. More detailed analysis of the kinetics of transcription using stopped flow in collaboration with the laboratory of Kenneth Johnson showed that the iodotyrosine variant produced a larger burst of short intermediate products characteristically made before the transition from the initiation complex to the elongation complex. Overall, these studies provide additional support for a model in which interactions between T7 RNA polymerase and its DNA template during initiation are changed by the nsAA substitution in a way that is apparently not possible with a normal amino acid.

BONNIE BARTEL, C-1309, Rice University. NOVEL PEROXISOMAL PROCESSES IN PLANTS.

Peroxisomes are subcellular compartments that sequester diverse, essential, and often oxidative reactions in eukaryotic cells. Although byproducts of these reactions undoubtedly damage peroxisomal components, almost nothing is known about how peroxisomes are degraded, and chemical tools to probe this process are lacking. We are screening for chemicals that modulate plant peroxisome destruction.

These experiments build on our discovery that autophagy of peroxisomes (pexophagy) occurs in the model plant, *Arabidopsis thaliana*, and is dramatically induced when a particular peroxisomal protease is dysfunctional. We are using bioassays exploiting unique aspects of plant peroxisome physiology to screen for lead compounds from arrayed chemical libraries that prevent peroxisome degradation. We also assayed an inhibitory compound identified by a collaborator in an in vitro autophagy assay for its efficacy in our seedling-based in vivo assay. We are examining various abiotic stressors that are known to promote degradation of other subcellular compartments to determine their impact on peroxisome turnover. In addition, we are examining pexophagy in various genetic backgrounds that influence peroxisome function. Compounds that inhibit either specific pexophagy or general autophagy will provide molecular probes with which to modulate the degradation of peroxisomes and other organelles and elucidate the molecular mechanisms of organelle dynamics.

MIKHAIL A. BELKIN, F-1705, The University of Texas at Austin. MID-INFRARED VIBRATIONAL NANOSPECTROSCOPY IN LIQUID ENVIRONMENT.

Following the year 2 development of evanescently-illuminated photoexpansion nanospectroscopy setup that produced nanoscale spectra of 20-nm-thick PMMA films in heavy water, we worked on improving the sensitivity of the setup down to a single molecular monolayer using encased atomic force

microscope cantilevers, instead of regular cantilevers. As discussed in the original proposal, the encased cantilevers were expected to yield at least 10 times improvement in sensitivity due to their higher mechanical Q- factor in liquid. Unfortunately, the encased cantilevers did not work as expected due to fabrication difficulties, water leakage, and parasitic photoexpansion signal and no good results were obtained. Thus, the results obtained in year 2 were not improved in year 3.

We also investigated a scattering-type near-field optical microscopy technique using a novel detection method based on observing small voltage oscillations in mid-infrared quantum cascade lasers produced by mixing of the optical field scattered by the metallized atomic force microscope tip with the field inside of the laser cavity. Initial results were obtained using 8.6 μm quantum cascade laser and reported at 2018 Conference on Lasers and Electro-Optics (CLEO) in May 2018. Imaging of a gold pattern mask on a sapphire substrate with 100-nm spatial resolution was demonstrated. We plan to use a similar detection method to extend this technique from a single-frequency imaging to spectroscopic imaging based on the principles of dual-comb spectroscopy during the next 3-year grant period.

MATTHEW R. BENNETT, C-1729, Rice University. THE ROLE OF PROTEIN/DNA INTERACTIONS IN THE KINETICS OF BIOCHEMICAL NETWORKS.

In the past year we have completed several new studies. We have recently completed our studies of how the binding affinity between DNA and sigma factors influence gene network dynamics. We have found that small mutations affecting sigma factor binding can determine how ligand-inducible transcription factors affect transcriptional initiation. In general, we showed that the regulatory range of a promoter (i.e. the difference between the maximum and minimum transcription rates) are drastically influenced by the sequences of the -10 and -35 sites of the promoter. A paper on this topic was published in Nature Communications. In another study, we experimentally showed that the timing of transcriptional signaling cascades can be highly variable and dependent upon initiation rates. Such cascades are important for cellular regulatory processes as they relay biochemical information from one genetic locus to another. We found that the rate with which the initial transcription factor is initiated determines not just the timing of the signal, but also its variability. This work was published in ACS Synthetic Biology. Other work that is currently submitted includes: 1) New results of our combined experimental and theoretical investigations of how promoters regulated by multiple transcription factors integrate the signals from each (in revision to ACS Synthetic Biology); and 2) Experimental work showing that molecular level details of biochemical reaction networks in single cells influences spatiotemporal patterning in populations (in revision at Nature Chemical Biology).

DAVID E. BERGBREITER, A-0639, Texas A&M University. MULTIPHASE MULTICOMPONENT SYSTEMS FOR SYNTHESIS AND CATALYSIS.

Our work this year was successful. One paper was accepted but is not yet published online. A second publication appeared in print since our previous report. The publication that was listed previously as accepted but had not been published described ways to use concepts of macromolecular chemistry to illustrate principals of NMR spectroscopy in the undergraduate curriculum. A publication that has been accepted but not yet published online describes initial ways to make phase-anchored cosolvents for PAOs from inexpensive PIB oligomers. The majority of our work this past year is unpublished and has focused on developing applications for the new nontoxic, sustainable hydrocarbon solvents we developed last year. The major results of that work has been to show that these poly(α -olefin)s (PAOs) can be modified by small amounts (ca 1 M) of polar cosolvents such that the environment of a dansyl or Nile Red solvatochromatic probe changes. The submitted paper describes work we carried out that used conventional alkanes and these new PAO solvents for SN2 chemistry. This submitted paper describes a fundamental study of SN2 reactions in alkanes, a solvent not previously studied for this very basic reaction and shows that reactions using a polyisobutylene (PIB)-bound phase transfer catalyst occur with rates like those effected by a similar catalyst in acetonitrile and that additions of small amounts of cosolvents accelerate these reactions' rates 10-fold. Second, we have begun studying the environmental applications of PAOs and related PIB-bound cosolvents, studying their application in water purification. Finally, we are exploring ways to use enthalpy driven processes to recycle and or degrade polyolefins including polyolefins we use as catalyst supports or cosolvents.

RICARDO A. BERNAL, AH-1649, The University of Texas at El Paso. DECIPHERING THE STRUCTURAL AND FUNCTIONAL BASIS FOR RING SEPARATION IN CHAPERONINS.

Misfolded proteins are associated with many well-known human diseases such as Alzheimer's disease, Parkinson's disease, cancer, cystic fibrosis, and other neuropathies, highlighting the importance of protein folding in human health. Protein folding is an important cellular process that depends on proteins reaching their native and fully functional three-dimensional structure. Cells have evolved macromolecular machines called chaperonins that specialize in maintaining cellular homeostasis by assisting proteins that have become misfolded. Protection provided by chaperonins is critical to support life since deletion of chaperonin genes from bacteria and yeast prove lethal. This past year, our studies have focused on two neurodegenerative disorders termed SPG13 and MitCHAP60 that have been linked to mutations in the human chaperonin hsp60. Although both disorders are neurodegenerative, they differ in the clinical symptoms presented and mode of inheritance. SPG13 is a member of hereditary spastic paraplegia (HSP) group of neurodegenerative diseases that are characterized by progressive weakness and spasticity (rigidity) in the lower extremities. MitCHAP-60 is an early-onset neurodegenerative disease inherited in an autosomal-recessive pattern characterized by neuronal hypomyelination and leukodystrophy (brain white matter degradation). To date, we have been able to determine the underlying cause of the MitCHAP60 and SPG13 diseases and an explanation for the mechanism of the neurodegeneration. Two important publications have resulted from work this past year, but one is still under review and will be reported next year. The other publication reports our initial results.

These Welch Foundation funded results have also been extensively reported at 16 occasions by the PI in invited seminars and in student oral and poster conference presentations. At all times, "The Welch Foundation (AH-1649)" is acknowledged.

W. E. BILLUPS, C-0490, Rice University. CHEMISTRY OF CARBON NANOMATERIALS.

As part of our interest in the functionalization of graphene, we have explored the Birch reduction as a route to the hydrographenes. The syntheses were carried out using lithium/ammonia as the reducing agent and tert-butyl alcohol as a proton source (Birch conditions). Different types of graphite were used as starting materials including synthetic graphite powder, natural flake graphite, and annealed graphite powder. The exfoliation process that we, and others, have investigated involves electron transfer into bulk graphite from intercalated lithium to yield lithium graphenide. Protonation of the graphenide yields hydrographene.

Analysis by solid-state ^{13}C NMR spectroscopy proved to be important since it was shown that the hydrographenes are composed of interior, isolated aromatic (predominantly fully substituted benzene) rings surrounded by saturated rings. The expected clusters of benzene rings were not found. NMR spectroscopy also offers strong evidence for the presence of tert-butyl alcohol and ethanol (workup solvent) that could not be removed in vacuo from the samples.

High-resolution transmission electron microscopy images revealed a remarkable change in morphology that results when hydrogen is added to the graphenide. The appearance of edge and circular dislocations and increased distances between graphitic layers are most visible in the case of the hydrographenes that are formed from annealed graphite. The repetitive hydrogenation of synthetic graphite powder leads to an increase in the distances between the graphitic layers in the (002) direction from 3.4 Å for the initial graphite to 4.11 Å after the first reduction and to 4.29 Å after a third reduction of the same material.

Defect-free graphite with classical spacing is formed when the hydrographenes are heated. The distance between carbon layers decreases from 4.11 to 3.44 Å after heating the samples to 1200 °C. This trend toward the classical spacing of graphite confirms the reversibility.

ERIC R. BITTNER, E-1337, University of Houston. THEORETICAL STUDIES OF ULTRAFAST AND COHERENT CHARGE-SEPARATION DYNAMICS IN ORGANIC PHOTOVOLTAIC SYSTEMS.

Over the last year, we have accomplished a key milestone in implementing a machine-learning-based approach for determining which nuclear motions, as described by normal motions, are most strongly coupled to intra-molecular state-to-state electronic transitions. We published a review article on this work in *Advances in Chemical Physics*. Moreover, we have developed and implemented a hybrid-quantum/classical methodology that treats the p-electronic degrees of freedom of a p-conjugated polymer ensemble as a fully interacting quantum sub-space coupled to a molecular-dynamics description of the nuclear motions. In Ref [2] we considered the role of interfacial disorder and p-stacking on the ability of an initially prepared excitonic state to dissociate into charge-separated electron/hole quasi-particle carriers. In our current implementation, the excitations are treated within the configuration interaction approximation. We are pushing this approach forward to include an explicit many-body time-dependent Hartree-Fock description which will allow for electronic relaxation and coherence effects to be considered on a self-consistent basis.

An important evolution/shift in our research is into the field of quantum optics. Here, we are developing fully quantum treatments of the radiation field coupled to fully-quantum dynamical treatments of molecular chromophore ensembles in microcavities. In resonant microcavities, the coupling to the radiation field cannot be treated perturbatively (as in our standard treatment of linear and non-linear spectroscopy).

Rather, one needs to treat the photon field and the material field on an equivalent basis. For this, we have developed an "input-output" theory which correctly couples the photons from an incoming laser field to the matter field and then returns emitted photons back to the outgoing radiation field.

PAUL BLOUNT, I-1420, The University of Texas Southwestern Medical Center. DETERMINING PROTEIN-LIPID AND PROTEIN-PROTEIN INTERACTIONS FOR A CHANNEL INVOLVED IN MECHANOSENSING.

The Y602C and R616Q mutations in TRPV4 cause skeletal dysplasia in humans. Therefore, we examined the channel activities of Y602C and R616Q mutants using the *Xenopus* oocyte expression system and two electrode voltage clamp, as well as the ability of these mutants to induce phenotypes in yeast. Our data indicate that Y602C and R616Q are both GOF mutations; such channel phenotypes may explain human genetic data. We then used disulfide trapping to determine proximity of these residues, and found that they easily form disulfide bridges, and that these appear to stabilize the closed state. In sum, these findings, as well as mutational data, are consistent with a cation- π interaction between Y602 and R516, which needs to be broken for channel gating; maintaining an interaction between these residues leads to normal gating, while destabilization of this interaction leads to increased channel activity and a GOF channel phenotype. We are now in the process of interpreting these data in the context of the crystal structures that have been obtained from different species.

JENNIFER S. BRODBELT, F-1155, The University of Texas at Austin. IMPACT OF CHARGES ON PROTEIN FRAGMENTATION.

One key goal is the development of new strategies to evaluate the structures of proteins. (1) We developed a method to deduce hydrogen bonding patterns in proteins based on ultraviolet photodissociation (UVPD) to monitor the fragmentation of intact protein ions. The engagement of the amide carbonyl oxygen of the protein backbone in hydrogen bonding was predicted based on the degree of hydrogen atom shifts in diagnostic fragment ions created by UVPD. The results correlated with the hydrogen-bonding motifs derived from molecular dynamics simulations and X-ray crystal structures. (2) Crosslinking was used to evaluate tertiary and quaternary structures of proteins. Crosslinks were identified using bis(sulfosuccinimidyl)suberate, a homobifunctional amine-to-amine crosslinker, and 4-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-methylmorpholinium chloride (DMTMM), a heterofunctional amine-to-carboxylic acid crosslinker.

UVPD and higher energy collision dissociation (HCD) provided a complementary panel of DMTMM crosslinks which extended the degree of structural insight obtained for the proteins. Differences in the types of unique DMTMM crosslinks were found based on the sizes of the products and charge states, with UVPD favoring the identification of larger species in higher charge states. (3) We developed a method for determining the collision cross sections of protein ions based on the decay rate of the time domain transient signal from an Orbitrap analyzer. A linear relationship between the pressure and the transient decay rate demonstrated that the signal decay was primarily due to ion-neutral collisions for protein ions. Coulombic repulsion between charge sites on multiply charged protein ions caused unfolding of the proteins. Many elements of protein tertiary structure were preserved in the gas phase for very low charge states. For higher charge states, tertiary structure was largely absent and secondary helical structures began to unfold as more charges are added.

MAURICE BROOKHART, E-1893, University of Houston. NEW Pd(II) AND Ni(II) CATALYSTS FOR OLEFIN POLYMERIZATIONS AND COPOLYMERIZATIONS.

During this grant period new Ni(II) and Pd(II) catalyst systems have been constructed and examined for polymerization/oligomerization of ethylene and copolymerization of ethylene with polar vinyl monomers. A brief description of each system investigated is outlined below.

1. A series of new cationic palladium catalysts based on phosphine-iminophosphorane ligands have been prepared and characterized using standard spectroscopic techniques together with structure determinations using X-ray diffraction studies. The effects of structural variations on polymerization of ethylene were investigated. The best catalyst was studied in detail. The most remarkable feature of the system is high thermal stability at 100C with a good productivity. (This work has been published in *Organometallics*.)

2. Work has been completed on the copolymerization of ethylene and vinyl triethoxysilane using diimine nickel catalysts. In-depth mechanistic studies have established the details of chain growth including the kinetic order in ethylene and comonomer, the catalyst resting state, the mechanisms of formation of branching in the polymer and the variation in polymer microstructures formed as a function of temperature and ethylene pressure. A convenient entry into the catalytic system from commercial activators has been developed and a provisional patent submitted on the process. This copolymer can be cross-linked to form PEX-b, a plastic used in making plumbing pipes and electrical cable coatings. The process developed here is an alternative to commercial processes. The catalyst system is highly active and efficient producing up to 550 Kg copolymer per g Ni. This work has been published in the *Journal of the American Chemical Society*.

3. An issue with late metal catalysts has been thermal stability. We have recently developed promising Ni catalysts supported by bidentate P,O ligands that exhibit exceptional thermal stability and are investigating their use in copolymerizations.

RICHARD K. BRUICK, I-1568, The University of Texas Southwestern Medical Center. ISOFORM-SELECTIVE REGULATION OF HIF-ALPHA BY ISOPRENOIDS.

We demonstrated that HIF-2 responds to metabolic perturbations in the isoprenoid biosynthetic pathway. For example, administration of geranylgeranyl transferase inhibitors (GGTI) leads to an isoform-selective induction of HIF-2 target genes in cultured cells and in vivo. Downstream analysis indicates that GGTI antagonizes the association of HIF-2a with DNAJA2, a member of a larger family of co-chaperones proteins that typically facilitate protein folding, transport, and assembly. DNAJA2 geranylgeranylation is required for its association with HIF-2a. To demonstrate that these effects are dependent upon the integrity of the HIF-2a PAS-B cavity, we introduced a cavity-filling S305M mutation within the HIF-2a PAS-B domain. This mutation reduces the binding affinity for both exogenous ligands and DNAJA2, while retaining proper structure and function of the domain. These data support a model in which geranylgeranylated DNAJA2 selectively interacts with HIF-2a in a cavity-dependent manner. We hypothesize that the prenylated tail of DNAJA2 may be inserted directly into the cavity. Pulldown assays and microscale thermophoresis analysis of purified PAS-B domains with prenylated peptides recapitulate the selectivity observed with intact proteins. Furthermore, loss of this interaction also changes the cytosolic localization of HIF-2a, blocking its recruitment to stress granules and subsequent recruitment into an alternative translation initiation factor complex. Lastly, we strengthened an association between HIF-2 and lipid metabolism by challenging mice with a high fat diet. While we observed no difference in weight gain in mice treated with a HIF-2 ligand on a standard chow diet, mice on a high fat diet gained less weight when given PT2399. These effects were not observed in mice bearing the drug resistant HIF-2a allele. We completed these studies prior to closing the laboratory in November 2017 and have submitted our findings for publication.

KEVIN BURGESS, A-1121, Texas A&M University. LADDER-RUNG MIMICS FOR PERTURBING PROTEIN-PROTEIN INTERACTIONS.

We have prepared a set of small molecules 1 that overlay three amino acid side-chains on beta-sheet motifs in proteins, like rungs on a ladder. Both solution and solid-phase methods have been developed.

These have been tested for inhibition of the protein-protein interaction between urokinaseplasminogen (uPA) and its receptor uPAR. Initial results from primary assays indicate some of these new molecules are inhibitors. Secondary assays are in progress. Fit of these molecules at the uPA•uPAR interface underlines applications of the Exploring Key Orientations (EKO) routine we developed earlier.

EKO was also used in the design of other minimalist mimics, this time to disrupt the interaction of PCSK9 with its LDLR receptor. PCSK9•LDLR is a key interaction in lowering cholesterol levels, validated by clinically used, and FDA approved, humanized antibodies, but for which there are virtually no published small molecule leads. This work was published as a full paper in *J. Am. Chem. Soc.* this year. As part of that work, we used a "cassette" for photoaffinity labeling that was developed in these labs specifically for the purpose (communicated in *ACS Med. Chem. Lett.*).

Other work impacted by our Welch funding this year, included research on 13-membered ring macrocycles as chemotypes for EKO in other applications, and work on fluorescent derivatives that disrupt TrkC•NT-3 as potential imaging agents in metastatic breast cancer.

SHAWN C. BURGESS, I-1804, The University of Texas Southwestern Medical Center. **DYSREGULATION OF INTERMEDIARY METABOLISM DURING DISEASE.**

Support from the Robert A. Welch Foundation was credited in 7 peer-reviewed research publications and 7 seminar lectures, including 2 international conferences (American Diabetes Association and the Obesity Society). The metabolomic and flux approaches (Ragavan et al. 2017) developed with Welch support contributed to a new understanding of body-weight regulation by novel hormone mechanisms (Lan et al. 2017), gastric bypass surgery (Pop et al. 2017) and the prevention of disease by altering mitochondrial pyruvate metabolism (Rauckhorst et al. 2017; Cappel et al. 2018; Wu et al. 2018). We investigated new roles for cataplerotic pathways in the small intestine (Potts et al. 2018), which we discovered contribute to intestinal lipid absorption and amino acid metabolism. These approaches also resolved the mechanism of an anti-cancer drug, which was found to have powerful effects on cellular redox state (Silvers et al. 2017).

We are currently extending metabolic modeling approaches to integrated mass spectrometry (MS) and nuclear magnetic resonance (NMR) data. This will allow us to examine metabolism on smaller tissue samples, and use these approaches in cell culture and in human clinical studies. One study coming to fruition in my lab describes how distal pathways of lipogenesis and gluconeogenesis can regulate each through energy sensing mechanisms. These experiments could not have been carried out without novel modeling approaches. Another study nearing completion describes the upregulation of oxidative metabolism in the liver of obese subjects with nonalcoholic fatty liver disease (NAFLD), hinting at potential interventions to treat this disease.

Finally, the postdoctoral fellow supported by the Welch Foundation (Dr. Stan Deja) was recruited to a faculty position in the UT Southwestern Center for Human Nutrition. Thus, Welch support also achieved its goal of supporting training for the next generation of scientists.

WALTER G. CHAPMAN, C-1241, Rice University. **STRUCTURE AND PROPERTIES OF COMPLEX FLUIDS IN THE BULK AND INTERFACIAL REGIONS.**

In 2017, three out of six papers that we published set forth new paradigms for calculating fluid properties; two papers also received special recognition. Some of these contributions are highlighted below.

We previously reported that enhanced water/alkane attraction is necessary to model solubility data. Our article in the Journal of Chemical Physics (JCP) demonstrates that polarizability and electrostatic interactions between water and alkanes, commonly ignored by conventional force fields, explain most of the effect. Our article was honored by an American Institute of Physics SciLight and was also the second highest rated University contribution on DOE's Basic Energy Sciences website for 2017. This research will be extended to other components.

A second article, that was chosen "Editors Pick" in JCP, demonstrates that fluctuations in solvation cannot be described within the macroscopic grand canonical framework, but requires a hierarchy of particle baths. This has broad implications for studying bio-macromolecular solvation.

In recent work, our unique cluster distribution theory replaces traditional distribution functions to describe multibody interactions. Our breakthrough is the first to predict accurately phase behavior of patchy colloids for arbitrarily shaped association sites, such as Janus and Saturn rings. Extension as a density functional theory (DFT) will explore self-assembled microstructure.

Other significant papers include: the first density gradient theory functional for amphiphilic molecules, prediction of how branching affects the phase behavior of mixed isomers, and prediction of the partitioning of mixtures between nanopores and the bulk using polyatomic DFT. Future results will use these methods to describe the effects of hyperbranched, bottlebrush, or copolymer architectures on partitioning of solutes between the bulk, permeable nanopores, and polymer-rich phases for chemical separations and drug delivery.

JAMES R. CHELIKOWSKY, F-1837, The University of Texas at Austin. **SIMULATING DIRECT IMAGES OF THE COVALENT BOND FROM ATOMIC FORCE MICROSCOPY.**

Over the past year, our work has continued to focus on simulating images of the covalent bond obtained from non-contact atomic force microscopy (nc-AFM). Our publications focused on two areas of work. One involved the simulation of different probe functionalizations. The other examined recently discovered graphene structures. One of our articles was selected as a feature publication.

In nc-AFM a scanning probe with an atomically sharp tip is rastered over the specimen of interest. If the tip probe is properly functionalized, e.g., using adsorbed CO, subatomic images can often be obtained. The mechanism for enhanced resolution using a CO tip is not well understood. We wish to understand the nature of this mechanism and predict whether other adsorbed molecules might also affect the resolution. To this end, we simulated measured images of benzene and dibenzo(cd,n) naphtho (3,2,1,8- pqra) perylene molecules with selected the probe tip modeled by CO, H₂, N₂, Br, and CH₂O. The probe tips so functionalized provide accurate simulations, save for the tip functionalized with a Br atom. CO and N₂ functionalized tips behave similarly, including producing contrast inversion with CO and N₂ tips at small tip heights.

In collaboration with an experimental group we examined atomically defined graphene nanoribbon (GNR) heterojunctions. GNR tunneling heterojunction represent a key element for the design of nanoscale electronic devices. The experimental work centered on the fabrication and electronic characterization of atomically precise GNR heterojunctions. These heterojunctions were characterized using bond-resolved scanning tunneling and atomic force microscopies, which enable chemical bond imaging at low temperatures. Scanning tunneling spectroscopy revealed that the band alignment across the heterojunction interface yields a type II heterojunction (or staggered gap interface), in agreement with our first-principles calculations.

BANGLIN CHEN, AX-1730, The University of Texas at San Antonio. FUNCTIONAL POROUS METAL-ORGANIC FRAMEWORKS FOR RECOGNITION OF SMALL MOLECULES.

With the support of the Welch Foundation, in this grant year we published 25 papers in Science, Nature Energy, J. Am. Chem. Soc., Adv. Mater., Coord Chem. Rev., Chem. Commun. and J. Mater. Chem. A. Some important progresses include ordered macro-microporous metal-organic framework single crystals (Science, 2018, 359, 206-210), and a flexible metal-organic framework with a high density of sulfonic acid sites for proton conduction (Nat. Energy, 2017, 2, 877-883). These works have significantly pushed forward the research on multifunctional metal-organic framework materials. We have realized the record materials for C₂H₂/C₂H₄ separation (Adv. Mater., 2017, 29, 1704210), methane storage (Adv. Mater., 2018, 30, 1704792), and hybrid membrane with high proton conductivity and low methanol permeability (Adv. Mater., 2018, 30, 1705155). We have also realized a microporous hydrogen-bonded organic framework from a metalloligand for highly efficient gas separation (J. Am. Chem. Soc., 2018, 140, 4596-4603), and a hybrid MOF membrane for highly selective gas separation (Energy Environ. Sci., 2017, 10, 1812-1819). I would like to take this opportunity to thank Welch Foundation for the generous and continuous support for my ongoing research.

CHUO CHEN, I-1868, The University of Texas Southwestern Medical Center. DEVELOPMENT OF ANTICANCER IMMUNOTHERAPEUTIC AGENTS.

In the previous grant period, we evaluated the activity of a DMXAA dimer and designed a new molecular scaffold for STING binding. Docking experiment suggested that the affinity of cyclo-[Gly-Gua-Gly-Ade] to STING is comparable to that of 2'3'-cGAMP. In this grant period, we developed a synthetic route to prepare this cyclic tetrapeptide. We further developed an in vitro assay to examine the interactions between small molecules and STING.

To solve the solubility issue associated with peptide synthesis, we adopted a solid phase approach to prepare the linear peptide precursor efficiently. We then performed macrocyclization in solution following cleavage of the linear tetrapeptide from the solid support. To evaluate its binding affinity toward STING, we exploited the enhanced thermal stability of proteins upon binding to a small-molecule ligand. We have confirmed that 2'3'-cGAMP, the endogenous STING ligand, stabilizes STING in a dose-dependent manner to prevent thermal aggregation. This assay can be carried out using lysates of THP-1 monocytes directly and coupled with proteomic analysis by mass spectroscopy to globally identify protein-drug interactions. This study has inspired a new direction of research in collaboration with Dr. Yonghao Yu also at UTSW to develop a technology platform for studying drug actions.

To demonstrate the feasibility of our synthetic and biochemical approaches, we first constructed cyclo-[Gly-Trp-Gly-Trp] as a model system. Based on results of our docking experiments, we expected cyclo-[Gly-Trp-Gly-Trp] to have an affinity toward STING in the low micromolar range. Surprisingly, we found that incubation of cyclo-[Gly-Trp-Gly-Trp] in THP-1 cell lysates led to destabilization of STING albeit at high micromolar to millimolar concentrations. We have also constructed the linear tetrapeptide Gly-Gua-Gly-Ade. We will examine its binding to STING after macrocyclization and study the interactions of these two cyclic tetrapeptides with STING.

ZHENG CHEN, AU-1731, The University of Texas Health Science Center at Houston. MOLECULAR MECHANISMS OF A CLOCK-ENHANCING NATURAL PRODUCT.

We previously identified NOB as a clock-enhancing molecule conferring potent protection against the metabolic syndrome (Cell Metabolism, 2016). We have made strong progress toward mechanistic understanding of the NOB-ROR axis. In a comprehensive study, we combined molecular and enzymatic assays with physiological and omics studies to reveal a pivotal regulatory role of NOB-ROR in mitochondrial respiratory chain (MRC) complexes. Specifically, we identified mechanistic functions of NOB-ROR in 1) MRC gene expression, 2) Complex II activity enhancement, and 3) MRC supercomplex architecture involving complex I and complex III. In accordance, we found that ATP production was enhanced in aged skeletal muscle while ROS amounts were diminished. These observations illustrate a cellular mechanism of NOB to promote healthy aging. This study has been submitted to a high-profile journal.

In another related study, we have identified cholesterol synthesis as a major biochemical pathway controlled by NOB-ROR. Analysis of both circulating metabolite and gene expression in liver provided strong evidence. Mechanistic studies are currently on-going to delineate the specific pathway linking NOB and cholesterol. Of note, oxysterols are known natural ligands for NOB. Our finding of NOB regulating cholesterol metabolism suggests an exciting feedback regulatory loop between circadian clocks and cholesterol metabolism.

In addition, we are continuing several related studies, including 1) ChIP-sequencing studies using anti-ROR antibodies, 2) structural studies of NOB interaction with ROR ligand binding domain, and 3) a novel mechanism role of NOB-ROR via PER2 protein degradation to enhance the amplitude of the circadian oscillator.

We published a number of papers during the past grant period acknowledging the generous support from the Welch Foundation. We expect to continue our excellent productivity in the following grant period.

ZHIJIAN J. CHEN, I-1389, The University of Texas Southwestern Medical Center. BIOCHEMICAL MECHANISM OF MAVS ACTIVATION BY PRION-LIKE POLYMERIZATION.

Viral infections induce type-I interferons through the detection of their nucleic acids by cytosolic sensors in infected cells. Viral RNA is recognized by the RNA sensor RIG-I or MDA5, which activates the mitochondrial adaptor protein MAVS. Upon activation, MAVS forms prion-like aggregates on the mitochondrial outer membranes. These aggregates are highly potent in activating the protein kinases IKK and TBK1, leading to induction of type-I interferons and other cytokines. For DNA viruses and other DNA-containing pathogens, their DNA is detected by the enzyme cGAS, which synthesizes cyclic GMP-AMP (cGAMP), a second messenger that binds and activates STING to induce interferons and cytokines. In the course of studying the MAVS aggregates, we

found that cGAS also forms puncta structures in cells transfected with DNA. Interestingly, these puncta behave as liquid droplets in that they are dynamic and can fuse with each other. We further investigated the mechanism of cGAS liquid droplet formation, and found that DNA binding to cGAS induces liquid phase separation, a physicochemical mechanism that underlies the formation of membraneless cellular compartments. The formation of cGAS droplets require multivalent interactions between cGAS and DNA. These results explain why long DNA is much more potent than short DNA in activating cGAS. The N-terminus of cGAS contains an unstructured and highly positively charged region that binds DNA, and this binding strongly facilitates liquid phase separation. The cGAS droplets function as microreactors in which cGAS, DNA and the substrates ATP and GTP are concentrated, greatly facilitating the production of cGAMP. We also discovered that zinc ions greatly enhance DNA-induced liquid phase transition of cGAS in cellular environments, suggesting that regulation of intracellular zinc ion concentration is another avenue of cGAS regulation. Thus, similar to MAVS aggregation, condensation of cGAS activates innate immune signaling.

CHENG-MING CHIANG, I-1805, The University of Texas Southwestern Medical Center. MECHANISTIC ACTION OF BET COMPOUND INHIBITORS IN CANCER THERAPEUTICS.

For Objective I, we analyzed p53-R280K gain-of-function mutant in MDA-MB-231 breast cancer cells and found that JQ1 treatment inhibits p53 mutant-regulated mevalonate cholesterol-synthesizing pathway by blocking recruitment of p53-R280K, BRD4, and SREBP-1a to the HMGCR1 and MVK gene loci in the mevalonate pathway. However, knockdown of BRD4 does not entirely recapitulate the effect of JQ1 treatment, indicating a potential involvement of other BET family proteins in the control of the mevalonate pathway.

For Objective II, we extended our studies to estrogen receptor alpha (ER)-regulated target gene transcription in MCF-7 breast cancer cells and found that DC-1 only selectively inhibits a subset of estradiol-dependent ER target gene transcription, unlike JQ1 that appears to broadly downregulate all estradiol-driven ER target expression. Using RNA-seq performed in BRD4-knockdown ER-positive nonmetastatic MCF-7 cells and also in ER-negative metastatic MDA-MB-231 breast cancer cells, we identified the matrisome network, which is an ensemble of extracellular matrix (ECM) and ECM-associated molecules, stands out as the top BRD4-regulated pathway in MDA-MB-231 cells.

Moreover, we found that 12 components in the matrisome network are overexpressed in invasive breast cancer as listed in The Cancer Genome Atlas (TCGA) patient sample database and many of them, e.g., Syndecan-4 (SDC4) and CST4, are potentially direct targets of p53, ER, and SREBP-1.

YUH MIN CHOOK, I-1532, The University of Texas Southwestern Medical Center. MECHANISMS OF IMPORTIN 8-MEDIATED NUCLEAR IMPORT.

Nothing is known about how Importin 8 (Imp8) recognizes cargos and little is known about Imp8 traffic in cells. One well-established cargo is the oncogenic eIF4E protein, which is both a translational initiation factor and a nuclear export adaptor for mRNAs. Although both active Imp8 and eIF4E proteins are challenging to purify, we have succeeded in obtaining milligram quantities of both. We assembled the Imp8-eIF4E complex for biochemical and crystallographic studies but the complex is currently not sufficiently stable in large quantities to enable crystallization. Many buffer conditions that are optimal for Imp8 are not optimal for eIF4E, and vice versa. However, we have finally identified conditions where the Imp8-eIF4E appears stable in small-scale gel filtration chromatography. The challenge for the next year is to scale up the assembly protocol to obtain sufficient material for crystallization screens. We have made very good progress in Aim 2 to solve the structure of Imp8 bound to RanGTP. We assembled the complex using full-length Imp8 and a C-terminally truncated Ran protein that is stabilized in the GTP-bound state, and the complex produces diffracting crystals. We will collect crystallographic data and solve the Imp8-Ran structure in the next few months. Finally, for Aim 3, we have generated tetracycline-regulated stable Hek293 cell lines of T-Rex-FLAG-Imp7, T-Rex-FLAG-Imp8 and T-Rex-FLAG-Imp9 to identify their respective potential cargos by co-immunoprecipitation/mass-spectrometry. This work will be done in collaboration with Mike Rout's lab at the Rockefeller University where we will use cryo-milling to preserve protein-protein interactions upon cell lysis. Imp7 and Imp8 share significant sequence homology. Structures of Imp8-eIF4E and Imp8-RanGTP will also inform heavily on the Imp7 system.

Similarly, structures of Imp7 complexes will also inform on the Imp8 system. Thus, we are pursuing proteomics studies of both Importin systems in parallel.

DAVID T. CHUANG, I-1286, The University of Texas Southwestern Medical Center. MITOCHONDRIAL SIGNALING BY REVERSIBLE PHOSPHORYLATION.

- In a collaborative study, Zucker fatty rats (ZFRs) were treated with the BDK inhibitor BT2 3,6-dichlorobenzo[b]thiophene-2-carboxylic acid (designated BT2) developed in the PI's laboratory. The increased BCAA flux through the BCKDC leads to significant lowering of BCAA and BCKA levels. These results are accompanied by reduced hepatic triglycerides concentrations and lower glucose and insulin levels. Unexpectedly, phosphoproteomics studies revealed that hepatic ATP-citrate lyase (ACL) is phosphorylated by BDK in vivo, which is attenuated by BT2 treatment. ACL is an important cytosolic enzyme in de novo lipogenesis and its phosphorylation on Ser454 is activating, leading to increased generation of acetyl-CoA for fatty acid synthesis. Adenoviral transfection of FAO cells with BDK markedly increases the phospho-ACL/ACL ratio. Our results describe a novel regulatory node involving both mitochondrial and cytosolic BDK in maintaining glucose, BCAA and lipid homeostasis.

- In a separate study, wild-type diet-induced obese (DIO) mice were treated with a liver-specific pan-PDK inhibitor 2-[(2,4-dihydroxyphenyl)sulfonyl]isoindoline-4,6-diol (PS10). Both PS10-treated DIO mice and PDK2/PDK4 double knockout (DKO) mice fed the same 60% high-fat diet (HFD) showed significantly improved glucose, insulin and pyruvate tolerance, compared to DIO controls. In response to lower glucose levels, cytosolic phosphorylated AMP-activated protein kinase (AMPK) in PS10-treated DIO and HFD-fed DKO mice is upregulated, accompanied by decreased nuclear

carbohydrate- responsive element binding protein (ChREBP), leading to markedly diminished hepatic steatosis in both study groups. Importantly, unlike DKO mice, increased hepatic PDC activity alone in PS10-treated DIO mice does not raise the ketone body level, compared to untreated DIO controls. The above findings provide a proof-of-principle that targeting hepatic PDKs alone is a novel therapeutic approach to treatment of obesity and T2D.

ABRAHAM CLEARFIELD, A-0673, Texas A&M University. SURFACE FUNCTIONALIZATION OF ZIRCONIUM PHOSPHATE AND PHOSPHONATE FOR DRUG DELIVERY, LUBRICATION, AND CATALYSIS.

ZrP Nanosheets Composite Hydrogel for Super-Loading Application.

A well-defined hydrogel was developed for super-loading of drug materials based on biocompatible PVA and ZrP nanosheets (PVA-ZrP hydrogel). PVA-ZrP hydrogels were prepared via a freezing- thawing cycle using mixture of PVA and exfoliated ZrP nanosheets. By adding ZrP nanosheets into PVA hydrogel, at mass ratio of 50:7 (PVA to ZrP), the loading capacity of drug material doxorubicin (DOX) at PVA-ZrP hydrogel was 20 times more than PVA hydrogel. Besides, the loading speed in the composite hydrogel is 8.6 times faster in 0.1mg/mL DOX solution compared to that in PVA hydrogel. The loading capacity of ZrP nanosheets here is 1.09 DOX per formula unit ZrP, which is 3.2 times larger than the loading capacity of layered ZrP. The loading capacity owing to not only the high surface areas of ZrP nanosheets but also the highly porous structure of hydrogel, both of which produce abundant loading space. ZrP nanosheets achieved the maximum loading capacity via the ion exchange with OH groups.

Besides hydrogels, ZrP nanosheets are capable to form microgels and films for drug loading/releasing as well. The polymer is not just limited to PVA either, various hydrophilic biomaterials including polyethylene glycol (PEG), polyvinylpyrrolidone (PVP) or gelatin are also good candidates to design the super-loading materials. Overall, we discovered that by engineering biocompatible ZrP monolayers into the traditional drug loading materials PVA, the loading capacity and speed were significantly increased. This would open a door for the research of drug loading, delivery and medical engineering.

CECILIA CLEMENTI, C-1570, Rice University. MAPPING THE FREE ENERGY LANDSCAPE OF PROTEINS BY COMBINING THEORY AND EXPERIMENT.

1) We have used a perturbative approach to show that protein size and topology play an important role in determining the response of protein dynamics to energetic frustration. In particular, we have shown how the dynamics of alpha-helical proteins are more susceptible to frustration than beta-sheet proteins of the same size. These results explain recent experimental findings and suggest that measuring the effect of frustration might be more successful with alpha-helical proteins. One paper is in revision.

2) We have developed and tested a Bayesian inference approach to integrating experimental data from multiples sources (FRET, NMR, mutagenesis, etc.) over multiple time and length scales into the definition of a molecular model. The model can be used to systematically test hypotheses on the physicochemical ingredients underlying a molecular process. We are applying this method to molecular systems that cannot be studied by any single experimental or computational technique alone. One paper has been published, and two are in preparation.

3) In order to obtain optimal coarse-grained potentials for macromolecules, we have used novel sparse- learning methodologies to extract coarse energy function from fine-grained simulation data. We have proved a theorem in this context and designed a practical application. One paper has been published, one submitted, and two are in preparation.

4) In order to assign an optimal resolution to a molecular model, we have proposed a systematic approach to learn a coarse representation from microscopic simulation data. We define effective coarse variables by identifying groups of atoms forming “coherent states” during the system dynamics. We have shown that this approach provides a revised view of the classical idea of pre-structured regions (foldons) in a protein folding process, suggesting a hierarchical characterization of the dynamics of molecular structures. One paper is published, and two additional ones are in preparation.

MELANIE H. COBB, I-1243, The University of Texas Southwestern Medical Center. REGULATORY AND CATALYTIC PROPERTIES OF MAP KINASE CASCADES.

We have analyzed the ERK2 cancer mutant, E322K. E322K generally displayed reduced stable substrate binding but increased binding to a handful of substrates in the presence of a MEK inhibitor, blocking pathway activation at a step prior to ERK phosphorylation. The explanation is not known; however, this property may contribute to the occurrence of this mutation in patients treated with Raf or MEK inhibitors. We crystallized another docking site mutant, D321N, and found it indistinguishable from wild type (rmsd 0.18Å). The stabilities of E322K and another activating mutation, the gatekeeper, are both decreased by 5 degrees, while D321N is stabilized by 5 degrees. We conclude that the docking site is an allosteric hot spot in ERK2. Mutation of ERK2 E322 to K causes altered substrate recognition, decreased activation threshold, increased nuclear localization, decreased stability, and slowed inactivation.

The protein kinases OSR1 and SPAK recognize RFXV motifs in WNKs and in their substrates. We developed a bioinformatic method to identify specificity determinants within and surrounding the RFXV motif (Taylor et al). To demonstrate the power of the method, we showed that two inwardly rectifying potassium channels, Kir2.1 and 2.3, not previously known to be regulated by the pathway, are in fact WNK1/OSR1 targets. Active OSR1 increases current carried by both channels, and mutation of the motif in Kir2.3 prevents channel activation by OSR1 (Fig. 4). Kir4.1, a related channel lacking the motif, was not affected. To determine how channel activity is increased by WNK1/OSR1, we used microscopy to show that Kir2.3 is restricted to a localization near the nucleus in the absence of OSR1 or in the presence of a WNK1 inhibitor. This information indicated that WNK1/OSR1 kinase activities are required to transport this channel, and most likely other channels and transporters, to the plasma membrane.

JEFFERY L. COFFER, P-1212, Texas Christian University. PROBING NEW CONFINED NANOSTRUCTURES AND ASSOCIATED INTERFACES WITHIN TUNABLE SILICON NANOTUBES.

In this third year of our most recent project, we have investigated the ability of silicon nanotubes (SiNTs) to control the structure and properties of selected metal nanocrystal frameworks organized along the nanotube surface. IN this regard, we have focused extensively on the formation of platinum (Pt) nanocrystals, with implications for nanocatalysis, electronics, and chemotherapeutics. Incubation of 3- (aminopropyl)triethoxysilane (APTES)-functionalized SiNTs in potassium tetrachloroplatinate (II) (K₂PtCl₄) solution under ambient conditions subsequently yields Pt nanocrystals with sizes ranging from 1-3 nm on SiNTs. From high-resolution transmission electron microscopy (HRTEM), nanocrystals with characteristic lattice spacings associated with Pt (d = 0.21 nm) are observed on the nanotubes. The amount of Pt deposited on SiNTs can be sensitively tuned from 20-60 wt% (characterized by TEM Energy Dispersive X-ray Analysis, EDX) by varying concentration of K₂PtCl₄ and immersion time in this Pt precursor. Through a series of careful control experiments, we have confirmed that the amine moieties of the functionalized nanotube surface play a key role in the mechanism of metal salt precursor reduction to the target nanocrystal.

These findings suggest a new approach to prepare Pt nanocrystals that are of potential benefit to a broad number of applications using pSiNTs as a template. Further investigations into the properties of the newly discovered Pt NCs-SiNT composites are underway to take advantage of this new synthetic methodology.

DON M. COLTART, E-1806, University of Houston. ASYMMETRIC CARBON-CARBON BOND FORMATION FROM FUNCTIONALIZED AZOALKENES.

We have been exploiting the putative 1,3-dipolar nature of in situ-derived 3-alkoxy-1-N-sulfonyl azopropenes and related intermediates (which has never before been described) as an access point to developing general and broadly applicable methods for the synthesis of chiral O- and N-heterocycles. In one application of our approach we developed a diastereoselective synthesis of β -fused bicyclic - lactones, an important class of chiral O-heterocycles, including those having quaternary centers. Both syn- and anti-fused bicyclic systems can be generated stereoselectively through a simple modification of the reaction conditions (Manuscript in press in Chem). We have developed a number of different approaches to chiral O- and N-heterocycles using 3-hydroxy-1-N-aryl/alkyl azopropenes and 3-amino-1-N-aryl/alkyl azopropenes, respectively, as 1,3-dipoles, which are new functional motifs developed by us that have reactivity properties similar to in situ-derived 3-alkoxy-1-N-sulfonyl azopropenes. The former systems have several substantial advantages. A very wide range of coupling partners can be conceived of for reaction development. The two approaches we have presently focused on use esters as the 1,3- dipole coupling partner. This gives highly substituted -lactones in the case of 3-hydroxy-1-N-aryl/alkyl azopropenes, and -lactams in the case of 3-amino-1-N-aryl/alkyl azopropenes, with excellent diastereoselectivity (manuscripts in preparation). Conditions have been developed in each case to allow access to either the syn- or anti-products, with complete stereochemical control. We are excited to continue to explore the reaction potential of these hitherto unknown functional arrangements in the context of a great many different dipole-dipole coupling reactions, which will undoubtedly lead to a wide range of useful chiral O- and N-heterocycles. (One publication has been published in 2017, one in 2018 and two have been accepted based on Welch support).

MARALICE CONACCI-SORRELL, I-1914, The University of Texas Southwestern Medical Center. NON-CANONICAL FUNCTIONS OF Myc IN PROTEIN ACETYLATION AND CHEMORESISTANCE.

Because Myc-nick binds acetyltransferases, we performed SILAC labeling and mass spectrometry and identified ~40 cytoplasmic proteins acetylated in a Myc-nick-dependent manner. Among them, we discovered several metabolic enzymes, including aldolase. In agreement, using metabolomics analyses we found that Myc-nick induces an increase in purines and their biosynthetic intermediates. We then developed an HPLC-Mass Spectrometry method to quantify the nucleotides identified in our metabolomics analyses as regulated by Myc-nick including: inosine, deoxyinosine, adenosine, and deoxyadenosine. We have now confirmed the metabolomics observations and determined that MYC- nick increases the levels of inosine and deoxyinosine and expanded these observations to multiple cell lines. Moreover, applying this method, we quantified inosine, deoxyinosine, adenosine, and deoxyadenosine in normal and colon cancer tissues from same patients and found that deoxyinosine is robustly upregulated in nearly all human colon cancer tissues. While investigating the molecular role Myc- nick-induced metabolites, we recently discovered that purines play a signaling role by directly activating mToc1 downstream of MYC-nick leading to an increase in global protein translation. These results compose a manuscript that is currently in preparation for submission in the Fall 2018.

Our findings support our hypothesis that MYC-nick-driven protein acetylation regulates metabolic pathways that control cancer progression. Moreover, our results propose that the combination of metabolomics and acetylome is a powerful approach in identifying pathways that mediated Myc-nick functions in cancer.

JACINTA C. CONRAD, E-1869, The University of Houston. STRUCTURE AND DYNAMICS OF ATTRACTIVE NANOPARTICLE GLASSES.

Nanoparticle glasses. We probed length-scale-dependent relaxations in nanoparticle glasses through the dynamics of tracer particles. Using molecular dynamics simulations, we examined the transport of noninteracting tracers in repulsive and attractive glassy liquids with identical long-time matrix diffusivities. Coupling of the tracer dynamics to collective relaxations in each matrix affected the shape of tracer trajectories, which were fractal within the repulsive matrix and more compact in the attractive (J. Phys. Chem. Lett. 2018). Scattering experiments on silica tracers in a glassy matrix of polystyrene particles revealed compressed exponential dynamics, indicative of stress relaxations, as well as two-stage aging behavior; tracers of distinct size coupled to

stress relaxations or diffused through the void network (in preparation). We developed a new aqueous model system to investigate repulsive and attractive glasses in confocal microscopy (Front. Phys. 2018), currently being adapted to scattering experiments. Crowded structure and dynamics. We probed the effects of macromolecular crowding on caged dynamics and solidification processes. Gold nanorods in solutions of non-adsorbing polymers were assembled into controlled open structures, which depended on the competition between depletion forces and transport rates and set by the polymer correlation length (ACS Appl. Nano Mater. 2018). Scattering and microscopy experiments revealed that the long-time dynamics of high-molecular-weight polymers grafted to the surface of nanoparticles were confined by neighboring grafted chains; addition of free polymers in solution compressed the grafted chains and enhanced their confinement (Macromolecules 2017).

Molecular dynamics simulations of nanoparticles diffusing in crowded polymer solutions revealed a new coupling mode between the nanoparticle and polymer center-of-mass, not accounted for in theories (Macromolecules 2018).

NICHOLAS K. CONRAD, I-1915, The University of Texas Southwestern Medical Center. **BIOCHEMICAL ANALYSIS OF A NOVEL S-ADENOSYLMETHIONINE SENSOR.**

We have made significant progress on the mechanisms of METTL16-dependent regulation of MAT2A. First, we have recently published a paper showing that the METTL16-dependent control of MAT2A RNA splicing occurs co-transcriptionally (Pendleton et al. 2018). This has important implications for the biochemical aspects of our studies in Aim 1. The METTL16-dependent co-transcriptional “decision” of whether or not to splice MAT2A must occur in a brief window in which hp1 has emerged from pol II but the RNA is not yet cleaved and polyadenylated. As such, the kinetic parameters are likely to be even more finely tuned than we had expected. Second, we have now entered a collaboration with Dr. Yunsun Nam’s lab. Her group is working on the structure of the complex between METTL16 and hp1 which reveals important aspects of METTL16’s biochemical properties. These studies are currently under revision.

While we have not yet faithfully recapitulated the MAT2A splicing in an in vitro splicing system, we continue to work toward this goal. We have expanded our studies of METTL16 in several important areas supported by our Welch foundation proposal. We have now shown that METTL16 is biochemically modified in cells by both methylation and phosphorylation in response to methionine starvation. Moreover, we have developed a GFP reporter system that enables us to define the factors that are important for METTL16-dependent MAT2A splicing. As expected after only one year, much work remains to be accomplished. However, these results support significant progress towards the goals of the Welch foundation proposal.

LYDIA M. CONTRERAS, F-1756, The University of Texas at Austin. **IN VIVO STRUCTURAL CHARACTERIZATION OF CATALYTIC AND REGULATORY RNAs.**

This year we made significant progress on our goals. We also started new collaborations to further enhance the impact our work is having. (1) We have successfully redesigned aspects of our technology platform to study regulatory and catalytic RNAs (i.e. tRNAs, Csr system) in three different organisms besides E.coli (*Z.mobilis*, *Shigella dysenteriae*, and *Mycobacteria smegmatis*); we have started a collaboration with the Krásny group at Czech Academy of Sciences to allow us intracellularly probing of RNAs under ranges of pH, temperature, oxidative stress to inform molecular responses to pathogenically-relevant stresses. (2) We have also redesigned and validated probes for the intracellular identification and characterization of RNA Thermometers in collaboration with the Murphy lab at Ohio University in the pathogenically relevant strain *Shigella dysenteriae*. (3) We have also optimized other molecular probing aspects of this work to evaluate the capacity to sense specific tertiary intermolecular interactions in vivo; this work has been performed in collaboration with a post-doctoral researcher at Stanford (Dr. Yesselman). Importantly, in these designs we are evaluating non-contiguous hybridization regions (formed by interacting tertiary structures, not contiguous in their primary sequence) to recognize long-range intramolecular RNA contacts in vivo. We have performed these experiments in the presence and absence of RNA helix proximity (due to presence/absence tetraloop (TL)-tetraloop receptor (TLR) of the well-characterized group I intron) in wild-type and TL-TLR mutant strains, respectively. We are currently working with Dr. Ren here at UT Austin to use this as a tool to confirm or refute specific long-range contacts in tertiary RNA structural characterization as another feature that will allow us to understand structural-functional catalytic relationships of RNAs. (4) We have also identified a number of novel factors that affect RNA function in vivo.

DAVID R. COREY, I-1244, The University of Texas Southwestern Medical Center. **RECOGNITION OF CELLULAR NUCLEIC ACIDS BY SYNTHETIC OLIGOMERS.**

We have made progress in several areas; 1) We used rigorous mass spectrometry to define proteins that interact with TNRC6 in mammalian cell nuclei, a critical protein involved in RNAi. Many of these proteins are known members of transcriptional control complexes. These findings provide a mechanistic bridge to understanding the molecular details of RNA-mediated control of transcription; 2) Fuch's dystrophy is a common inherited eye disease affecting up to four percent of the US population. Half of these cases are at least partially linked an expanded trinucleotide repeat within the TCF4 gene. We developed synthetic oligonucleotide inhibitors to block this repeat and reverse some cellular symptoms associated with disease; and 3) We have continued to expand the range of synthetic compounds available for activating expression of frataxin as a potential treatment of Friedreich's Ataxia.

GREGORY CUNY, E-1916, University of Houston. **SYNTHESIS OF CONFORMATIONAL RESTRICTED NATURAL PRODUCTS.**

We have completed a synthesis study of (–)-noroliveroline and related stereoisomers, as well as demonstrated that one isomer is a potent beta-1/beta-2 adrenergic receptor antagonist. This study is significant since it supports our scientific premise that conformational restricted natural products (and derivatives) can be used to define binding modes of macromolecules that are difficult to study by other means (e.g. co-crystallization). A paper describing this work was published earlier this year. We are also completing the synthesis of 8-phenoxy aporphines, which represents an interesting and unexplored (both with

respect to synthesis and bio-activities) subset of natural products. We anticipate publishing this work in the coming year. We have made progress in our approach to the biaryl spirocyclic ether gymnothespirolignan A. Namely, we have achieved a synthetic route to key precursors for the synthesis of fluoren-9-ones and/or fluoren-9-ols, albeit in low yield. The current route is being optimized in order to provide sufficient material to explore their cyclization using mono-ligated Pd catalyzed ortho-phenol arylation. We also initiated our synthetic approach to the pentacyclic alkaloid pallimamine. However, attempts to generate 4,4-dialkyl-3-isoquinolinones using a carboacetoxylation via direct C-H bond functionalization did not proceed as expected. But interestingly, during the course of this study we discovered a new synthesis of 5,5-disubstituted oxazolidine-2,4-diones utilizing an oxidative cyclization reaction. We have optimized the reaction, explored its substrate scope and are currently completing an illustrative application. In addition, we are determining the stereochemical course of the reaction, which will provide insight into the reaction mechanism. This work will be presented at the American Chemical Society National Meeting in August 2018. We also anticipate publishing these findings. We are now exploring several alternative routes.

PENGCHENG DAI, C-1839, Rice Univer

sity. TRANSPORT, MAGNETIC, AND NEUTRON SCATTERING STUDIES OF QUANTUM MATERIALS.

During the current grant year from June 2017 till June 2018, our group published 12 papers describing our progress in studying spin dynamics in QMs. This includes the discovery of a novel dynamic spin- lattice coupling in NaFeAs, a novel spin-lattice coupling in YIG, and other interesting papers on spin dynamics of iron based superconductors.

KEVIN N. DALBY, F-1390, The University of Texas at Austin. TARGETING MELK FOR CANCER THERAPY.

In this grant period we have delineated the kinetic mechanism of binding of novel indolinone inhibitors to MELK using fluorescence stopped-flow. We have identified compounds that bind tightly (K_i of 90 pM) and slowly (residence time greater than 12 minutes). We determined that a relatively non-conserved residue Glu93 of MELK is important for the observed slow binding, potentially mediating a conformational change that may be exploited to improve specificity of binding. Using a BRET assay, we established the IC50 for the targeting of MELK in mammalian cells by compound 17 ($K_i=223$ pM) is 13 nM. Studies are underway to improve the bioavailability of lead analogs by incorporating bioisosteres of a hydrolysable carboxymethyl ester.

GAUDENZ DANUSER, I-1840, The University of Texas Southwestern Medical Center. PROBING ONCOGENIC FUNCTIONS OF VIMENTIN FILAMENTS BY SMALL MOLECULE SCREENS.

As reported last year, we have identified SW104004 and SW123626 as two compounds acutely perturbing VIF network integrity. Especially SW123626 seems to depolymerize VIF without wholesale effects on overall cytoskeleton organization. Our current goals are validation of the compound effect in several VIF-related cell functions plus identification of the mechanism of action. Towards the former goal, we have developed a fast 3D imaging assay to probe cell proliferation and survival of individual cells in single cell and spheroid culture in physiologically relevant microenvironments *ex vivo*. A paper describing the method is currently under review. The assay is not limited to EMT models and VIF function but permits drug response analysis of a broad palette of cancer models. Accordingly, this method is used in several projects in the lab, e.g. to test the differential drug sensitivity of melanoma with distinct mutational profiles. Second, in collaboration with Daniel Irimia's lab at MGH, we developed a microfluidic device to probe various parameters of cellular chemotaxis. This assay is inspired by two studies we published in 2016/17, which defined VIF as a cell polarity persistence factor. Hence, VIF enhances directionality of chemotactic migration in presence of noise, however also generates inertia during gradient switches. Our microfluidics chamber permits gradient switches on a time scale of 30s concurrent with wash-in and wash-out of drug compounds. This will allow us to functionally characterize the two compound in the context of directed cell migration. The experiments are ongoing. We will also revisit some of the other 14 compounds from our initial screen that affect VIF organization, but less specific. Finally, we have generated a panel of mesenchymal cell lines that carry mutations in VIF's numerous phosphorylation sites. Using these in combination with the identified compounds will allow us to make a first step towards mechanism of action.

DONALD J. DARENSBOURG, A-0923, Texas A&M University. DESIGN AND REACTIVITY STUDIES OF METAL CATALYSTS FOR THE PRODUCTION OF POLYCARBONATES FROM NOVEL OXIRANES AND CARBON DIOXIDE.

During the funding period we have analyzed the extent to which renewable resources can provide epoxies for the production of polycarbonates by copolymerization with carbon dioxide. Specifically, the use of renewable resources that are not competitive with food production was emphasized. The further development of methods for the synthesis of polycarbonate polyols of well-defined molecular weights and polydispersities has been carried out using a wide range of oxirane monomers. Specifically, we systematically studied the reaction activity and blocking efficiency of various macro-chain transfer agents, including PEG and PPG. We have incorporated this process for the preparation of the first CO₂-based production of a polycarbonate with the ability to autonomously self-heal. This polymer was synthesized via a one-pot strategy involving in tandem three different catalytic processes, hydrolysis of epoxides, immortal copolymerization of CO₂/epoxides, and thiol-ene click reactions.

MARCEY Y. DARENSBOURG, A-0924, Texas A&M University. FUNDAMENTAL CHEMISTRY THAT CONTROLS NITRIC OXIDE RELEASE, CAPTURE, OR RETENTION IN THE DINITROSYL IRON UNIT.

We relate the fundamental chemistry of the Fe(NO)₂ unit to its stability and potential NO storage or NO-releasing ability. In collaboration with Dr. Soon Mi Lim, Prof. Karen Wooley's laboratory, we explore the potential of Fe(NO)₂ derivatives to serve as a source of NO and ROS to endothelial and smooth muscle cells. The influence of added copper to mediate NO release from DNICs further defines therapeutic potential. We showed that sugar-appended

thiols enhance interaction of DNIC's with endothelial and smooth muscle cells. Confocal microscopy and a decrease in expression of pMLL2 (Western blot assay related to SMC relaxation) are consistent with NO delivery that is promoted in the presence of copper.

Major electrocatalysis studies drew on synthetic efforts in iron nitrosyl complexes resulting in PNAS (M258) and Chemical Science (M257) publications. Invited lectures and contributions (such as the DOE report, Science (M259)) honed our interpretation of these results and led to a holistic understanding of catalysts that guide H₂ formation from strategically placed acid/base pairs and proton/hydride coupling. Alternatively, as in nitrogenase, with sufficient delocalization of charge, reductive elimination results from adjacent metal hydrides. Our efforts provided opportunity to install redox-active NO ligands on adjacent metal sites; an Fe(NO) within a N₂S₂ ligand field that permits attachment, via thiolate sulfurs, to a redox-active Fe(NO)₂. The subtle interplay of redox potential, proton affinity, and proton/hydride coupling provides key features of molecular proton reduction electrocatalysts. Biomimetic studies of cyanide as a docking agent demonstrated the utility of the redox-active iron dinitrosyl receiver unit in design of complexes that display linkage isomerism of the ambidentate CN- ligand (M260). In JACS (M261), a more extensive study connected CN docking and linkage isomerism in synthetic analogues of artificial [FeFe]-hydrogenase maturation.

BRYAN W. DAVIES, F-1870, The University of Texas at Austin. HIGH-THROUGHPUT SCREENING FOR DISCOVERY AND DEVELOPMENT OF ANTIMICROBIAL PEPTIDES.

We continue to advance all research objectives of this proposal. Our flagship manuscript was accepted to Cell in January 2018. Multiple media outlets including magazines, television news, and radio shows have covered our story. The technology supported by this grant and described in our paper forms the foundational technology of a new biotech startup; Anexigen Therapeutics. Anexigen opened June 2018. The goal of Anexigen is to use our approach and new understanding of peptides to develop the next generation of antibiotics for clinical testing. Early support from Welch was critical in developing our scientific understanding of antimicrobial peptides that has matured to the industrial space in 3 years.

We continue to explore new amino acid motifs we have identified for their antimicrobial action. A particular tetramer motif appears to help peptides differentiate bacteria based on differences in their cell surface. We are proceeding to characterize this motif and the cell surface structures it recognizes.

The results from our large (~1 million) peptide screening campaigns have provide a wealth of information on amino acid sequence and structure with antimicrobial activity. We are mining these datasets to identify rules for designing new peptides libraries with enhanced antimicrobial properties. In particular we are focusing on the development of cyclic two stranded beta-sheet peptide scaffolds. This structure provides enhanced rigidity, improved target interaction, and ability to traverse the bacterial cell envelope. New libraries based on this scaffold are being constructed for screening.

JEF K. DE BRABANDER, I-1422, The University of Texas Southwestern Medical Center. SYNTHESIS AND CHEMICAL BIOLOGY OF BIOACTIVE SMALL MOLECULES.

During the past year, we made significant progress (5 published papers) on a variety of fronts. Related to our interest in complex natural products, we have completed the synthesis of the complex sugar fragments of fidaxomicin, as well as the fragments required to assemble its macrocyclic core structure. We envision to complete a total synthesis during the coming grant year, which will lay the foundation to improve the physicochemical properties of this non-systemically available antibiotic. The ultimate goal is to achieve systemic bioavailability as an entry to the potential treatment of multi-drug resistant tuberculosis. Related to our medicinal chemistry programs, we focused on novel leads for the treatment of Human African Trypanosomiasis by selectively targeting the parasite isoform of S-adenosylmethionine decarboxylase, an enzyme in the polyamine biosynthesis pathway. We also have made great strides in optimizing a novel lead series for the potential treatment of the devastating brain cancer glioblastoma multiforme. Through a High Throughput Screening campaign, we identified a benzimidazolium compound that specifically target the tumor-derived neuronal stem cells (Mut 6 cells) that define the stem-cell population of glioblastoma. We have now prepared over 300 analogs within this series that help define the structure- activity relations within this series and led to potent nanomolar analogs that are metabolically stable in vivo. We also prepared probe-reagents for mode-of-action studies, that in collaboration with Dr. Luis Parada at the Memorial Sloan Kettering Cancer Center led to the identification of a unique effect of respiration-coupled oxidative phosphorylation that is selectively lethal to Mut 6 brain cancer stem cells but not to normal astrocytes or mouse embryonic fibroblasts. We recently submitted a full paper under review by the journal "Nature" on the mode-of-action, effects on oxidative phosphorylation, and antitumor effects in vitro and in vivo.

RALPH J. DEBERARDINIS, I-1733, The University of Texas Southwestern Medical Center. COMPARTMENTATION OF A REDOX-BALANCING METABOLIC ACTIVITY IN THE CANCER CELL PEROXISOME.

To understand redox metabolism in human cancer, we performed intra-operative infusions with ¹³C- labeled nutrients in two cancers with different redox states and tricarboxylic acid (TCA) cycle activity. In clear cell renal cell carcinoma (ccRCC), we infused patients with [U-¹³C]glucose during surgical tumor resection and analyzed ¹³C labeling in metabolites extracted from the tumors and adjacent kidney. We found that the tumors excessively labeled glycolytic intermediates but had poor labeling in TCA cycle intermediates, suggesting high rates of glycolysis but reduced glucose oxidation (the "Warburg effect"). Importantly, loss of the tumor suppressor VHL, which is functionally inactivated in 80-90% of ccRCCs, is sufficient to induce the Warburg effect in cultured cells, providing a plausible mechanism for suppressed TCA cycle activity in vivo. The human data are also consistent with our observation that ccRCCs have a low NAD⁺/NADH redox ratio, consistent with elevated glycolysis and/or suppressed mitochondrial respiration. Experiments in year 3 will attempt to determine the mechanism for these redox disturbances. Second, we analyzed fuel metabolism in non-small cell lung cancer (NSCLC). Our previous work (Hensley CT et al, Cell 2016; 164:681-694) revealed that these tumors enhance TCA cycle metabolism relative to adjacent lung, and that the tumors consume other fuels in addition to glucose in vivo. This year, we identified lactate as a carbon source for TCA cycle metabolism in lung cancer, both in

humans and in mice. We reported that lactate's contribution to the TCA cycle exceeds that of glucose, particularly in tumors localized to the lung. This finding contrasts with the old view that the Warburg effect dominates tumor metabolism; indeed, of the several forms of human cancer we have analyzed using ^{13}C tracers, only ccRCC exhibits strong evidence of the Warburg effect. Our findings in NSCLC were published in Cell (Faubert B et al, Cell 2017; 171:358-371).

MICHAEL W. DEEM, C-1917, Rice University. DESIGN OF NOVEL ORGANIC STRUCTURE DIRECTING AGENTS FOR ZEOLITES.

We have completed the first task [Proc. Natl. Acad. Sci. USA 114 (2017) 5101]. Zeolite and zeolite-like molecular sieves are being used in a large number of applications such as adsorption and catalysis. Achievement of the long-standing goal of creating a chiral, polycrystalline molecular sieve with bulk enantioenrichment would enable these materials to perform enantioselective functions. Here, we report the synthesis of enantiomerically enriched samples of a molecular sieve. Enantiopure organic structure directing agents are designed with the assistance of computational methods and used to synthesize enantioenriched, polycrystalline molecular sieve samples of either enantiomer. Computational results correctly predicted which enantiomer is obtained, and enantiomeric enrichment is proven by high-resolution transmission electron microscopy. The enantioenriched and racemic samples of the molecular sieves are tested as adsorbents and heterogeneous catalysts. The enantioenriched molecular sieves show enantioselectivity for the ring opening reaction of epoxides and enantioselective adsorption of 2-butanol (the R enantiomer of the molecular sieve shows opposite and approximately equal enantioselectivity compared with the S enantiomer of the molecular sieve, whereas the racemic sample of the molecular sieve shows no enantioselectivity). We have started on the second task. Suitable forcefields have been identified for charged zeolites and OSDAs.

H. V. RASIKA DIAS, Y-1289, The University of Texas at Arlington. METAL COMPLEXES OF HIGHLY FLUORINATED LIGANDS.

Iron pentacarbonyl is a molecule with a long, rich history. It most typically undergoes CO replacement chemistry and serves as a Lewis acid. We have uncovered molecules that display rare Lewis basic properties of $\text{Fe}(\text{CO})_5$. For example it coordinates to Lewis acidic silver and gold fragments leading to heterobimetallic Fe-Ag and Fe-Au compounds such as $[\text{B}\{3,5\text{-(CF}_3\text{)}_2\text{C}_6\text{H}_3\}_4]\text{AgFe}(\text{CO})_5$ and $[\text{Mes}_3\text{PAu-Fe}(\text{CO})_5][\text{SbF}_6]$. Weakly coordinating anions like $[\text{SbF}_6]^-$ and $[\text{B}\{3,5\text{-(CF}_3\text{)}_2\text{C}_6\text{H}_3\}_4]^-$ play a key role in this work. Structures, chemistry and bonding of these molecules were reported. We have also investigated the chemistry of fluorinated pyrazolates with zinc(II) and isolated for the first time, several dinuclear zinc(II) adducts supported by such ligands, e.g., $[\{(3,5\text{-(CF}_3\text{)}_2\text{Pz})\text{ZnEt}\}_2(\mu\text{-THF})]$. These compounds mediate olefin aziridination chemistry very effectively, in contrast to the analogous non-fluorinated zinc(II) adducts. This work illustrates the effective use of earth friendly zinc in olefin aziridination applications. We have also worked on a new dianionic, bis(borylamido)naphthalene ligand, which allows the isolation of overall neutral metal adducts with Zn(II) ions. Stabilization of rare zinc-isocyanide complexes using this ligand support was reported.

LOI H. DO, E-1894, University of Houston. SITE-DIFFERENTIATED PLATFORMS FOR OLEFIN POLYMERIZATION CATALYSIS.

During the 2017-2018 funding period, our lab has achieved the following: 1) demonstrated that PEGylation of conventional metal catalysts is an effective strategy to create new binding sites for secondary cations; 2) shown that heterobimetallic palladium-alkali complexes are excellent catalysts for ethylene and alkyl acrylate copolymerization; and 3) performed preliminary mechanistic studies of ethylene/methyl acrylate copolymerization reactions. Building on our prior work on the nickel phenoxyimine systems, we extended our strategy to install polyethylene glycol (PEG) chains to other classes of olefin polymerization catalysts. We have successfully prepared PEGylated variants of palladium phosphine-phosphonate and nickel phosphine-phenolate complexes. Excitingly, we found that the addition of alkali salts to these compounds provided discrete heterobimetallic species that are remarkably active catalysts for ethylene homopolymerization. Our molecular constructs provide opportunities to investigate the reactivity of uncommon heterobimetallics, such as transition metal-lanthanide compounds in future work. In our second achievement, our lab has demonstrated that palladium-alkali phosphine phosphate complexes are capable of copolymerizing ethylene and alkyl acrylates with greater rates and at higher temperatures than conventional monopalladium catalysts. Notably, the increase in catalyst activity did not lead to reduction in polymer molecular weight. We anticipate that further steric/electronic optimization of our palladium-alkali compounds will lead to even greater catalytic performance. Finally, we have carried out mechanistic studies to evaluate the effects of alkali ions on the reaction of our Pd (P,O-ligand) complexes with ethylene and methyl acrylate. We have prepared Pd(P,O-ligand)(methyl acrylate) species and are using it as a model compound to study the insertion of ethylene into palladium-alkyl bonds in both the presence and absence of sodium ions.

SHEEL DODANI, AT-1918, The University of Texas at Dallas. EXPLORING THE NEGATIVE (X-) SIDE OF BIOLOGY: MOLECULAR AND PROTEIN-BASED TECHNOLOGIES FOR IMAGING CELLULAR CHLORIDE.

We have generated a family of turn-on fluorescent rhodopsin chloride sensors based on the proton-pumping rhodopsin from *Gloeobacter violaceus* (GR). To generate a starting point, all possible amino acid substitutions at the counterion position D121 were sampled using site-saturation mutagenesis.

Mutant proteins were readily expressed and screened in live *E. coli* using a fluorescence plate reader assay in buffer at saturating chloride concentrations. A single point mutant variant from aspartate to valine shows a 2-fold fluorescence turn-on at pH 5. GR D121V does not pump protons or chloride, but only senses chloride with a K_d of 105 mM. Moreover, no interference is observed in the presence of abundant anions like phosphate and sulfate. We have also confirmed the properties of GR D121V at the single cell level with flow cytometry and confocal microscopy in live *E. coli*. Properties are also maintained in purified protein (manuscript in preparation). With this starting point in hand, we have explored two different protein engineering strategies to improve GR D121V. In one approach, we have used direct coupling analysis methods with Professor Faruck Morcos at UTD to predict the order in which site-saturation mutagenesis should be carried out and have generated the sensor GR D121V/E132K/A84K/T125C/V245I. It has a larger dynamic range in live *E. coli* with a 6-fold increase in fluorescence intensity at pH 5 with a K_d of 84 mM (manuscript in preparation). In parallel, we have used random mutagenesis to

generate large libraries of sensors and screened these in lower chloride concentrations. With this approach, we have discovered the sensor GR G16E/D121V/Y163N/G261A that shows a 2-fold turn-on with a significantly lower K_d of 11 mM at pH 5 (manuscript in preparation). We are confident that our methods will generate a sensitive and pH independent sensor with an even larger dynamic range for imaging chloride dynamics in mammalian cells.

ANDREAS DONCIC, I-1919, The University of Texas Southwestern Medical Center. INVESTIGATING CELL FATE DECISIONS DURING YEAST SPORULATION USING LIVE SINGLE CELL METABOLITE MEASUREMENTS.

Aim 1: The Doncic lab has developed a new tools to study how metabolic inputs affect cell decision- making, including: i) a budding yeast meiosis/quiescence model for cell fate decision-making, ii) six-color simultaneous quantitative fluorescence imaging; iii) a mathematical method, called ‘statistical evidence’ for rigorously converting information from multiple fluorescently tagged markers into cell fate probabilities and iv) multiple yeast strains engineered to express 6 markers endogenously tagged on a single allele: two markers allow cell fate and cell cycle activity to be monitored, 4 allow tracking of distinct metabolic parameters. Different strains were imaged over a 50h period while growing in microfluidic chambers and undergoing several cycles of mitosis before entering either meiosis or quiescence. In combination, these tools have allowed them to translate information from a large combination of measurements into individual cell fate probabilities with very high precision. They showed that cell fate decisions can be largely deterministic and that cells can decide their future fates long before commitment mechanisms are activated, indeed even before birth. Moreover, their findings strongly suggest that the meiosis/quiescence fate is controlled by the metabolic status of the cell, which could be directly related to the levels of intracellular nutrients/metabolites. This work was recently accepted for publication in Mol. Cell.

Aim 2: Current effort is direct towards comparing single-cell readouts of the expression levels of the enzymes involved in trehalose storage and consumption (Tps1/Nth1, respectively) and those involved in glycogen storage and consumption (Gsy2/Gph1, respectively) with biochemically measured levels of trehalose and glycogen. Preliminary results confirm their correlative power. These experiments will be continued to determine the specific requirements for carbohydrate reserves as inputs into the meiosis/quiescence cell fate decision.

IVAN D'ORSO, I-1782, The University of Texas Southwestern Medical Center. COOPERATIVE ASSEMBLY OF HIV TRANSCRIPTION ELONGATION COMPLEXES.

The transcriptional program of HIV is controlled at the elongation step by an RNA polymerase II (Pol II) complex that pauses at the promoter shortly after transcription initiation. Pol II pause release and conversion into the productive elongating form is sequentially activated by master transcription factors (TFs) that promote recruitment of the host CDK9 kinase, which phosphorylates paused Pol II to support viral transcription and replication. Previous paradigm-shifting discoveries from my lab have led us to propose a model whereby CDK9 is recruited to the viral promoter early in the transcription cycle as part of the 7SK complex in which the kinase remains catalytically inactive. During years 1 & 2 of The Welch Foundation award, we used a combination of genetic and biochemical approaches and discovered that the transcriptional regulator KAP1/TRIM28 bridge the CDK9-7SK complex to the promoter containing paused Pol II to facilitate “on-site” kinase activation and transcriptional pause release. During year 3, we have made remarkable progress towards achieving the Specific Aims of this proposal. For Specific Aim 1, we discovered that KAP1 uses its tandem plant-homology domain (PHD)-bromodomain (BD) [PHD- BD domain] to contact unmodified histone 4 (H4) tails to assemble on chromatin at the viral promoter.

This protein-peptide interaction facilitates the proper assembly of Pol II at the viral genome as well as recruitment of the elongation complex to promote transcription activation. For Specific Aim 2, we demonstrated that while KAP1 is needed for gene activation by inducible cellular TFs such as NF-kappaB, it is dispensable for activation by the HIV TF Tat, thus indicating unique evolutionary strategies by which HIV robustly activates its genome (bypassing a host cell regulatory mechanism). Ongoing studies are in progress to fully determine the mechanisms of assembly using a biochemical-biophysical approach and define the molecular bases for the viral evolved circuit.

PETER DOUGLAS, I-1920, The University of Texas Southwestern Medical Center. STRESS-MEDIATED ACTIN PHOSPHORYLATION IN ENDOCYTOSIS AND INTESTINAL BARRIER FUNCTION.

We have made substantial progress on the respective aims established in our original proposal. As a result, we will be submitting a manuscript on this proposed work for review at a peer-reviewed scientific journal review in the next few months. Regarding Aim 1, we have identified two potential serine phosphorylation sites with ACT-5. We had initially suspected that the phosphorylated residue was a tyrosine. However ACT-5 immunoprecipitations subject to liquid chromatography mass spectrometry detection identified serine residues at position 232 and 239. We are presently generating single point mutations within both residues to determine the biological significance of both sites. Additionally, we completed a candidate-based RNAi screen of all the kinases and phosphatase, which were identified in complex with ACT-5. With the next year, we plan to have identified the kinase and phosphatase, which both acts on ACT-5 and is subject to regulation by HSF-1. Regarding Aim 2, we have modeled the respective phosphorylation sites on existing crystal structures of F-actin and discovered that the S232 but not S239 resides within the troponin binding site of ACT-5. Troponin acts to stabilize filamentous actin bound to tropomyosin so we speculate that mutations that mimic a phosphorylated serine at position 232 of ACT-5 will destabilize the actin network in the intestine and cause early onset decay of the intestinal epithelia. We have just begun to examine links between ACT-5 and the endocytic recycler, RAB-11.1 and anticipate having data to report in the next progress report. Overall, we have made significant progress on our two aims and anticipate a strong paper being in press regarding this work for the next progress report.

MICHAEL C. DOWNER, F-1038, The University of Texas at Austin. FEMTOSECOND OPTICAL PROBES OF NANO-INTERFACE CHEMISTRY.

Our Welch-sponsored research employs a diverse suite of optical methods to probe chemistry of micro- and nano-interfaces noninvasively. For the past few years, we have used dark-field microscopy with deeply penetrating near-infrared light to characterize natural bulk microstructure in bitumen and to elucidate its connection to micro-mechanical properties of pavement-grade binders. This year we published a new study [Ramm et al., *J. Microscopy* (2018)] showing that microstructural kinetics following a fast 20 C temperature increment correlated quantitatively with time-variations in shear modulus. We developed a model of a colloidal suspension of micro-spheres embedded in a uniform matrix to explain both optical and rheological data. The results help to develop predictive micro- mechanical models of composite strength. We published three new studies that use optical second- harmonic generation (SHG) to probe crystal structure [Zhou et al., *Nano Lett.* 17, 5508 (2017)], polarization retention kinetics [Cho et al., *Appl. Phys. Lett.* 112, 162901 (2018)], and temperature- and composition-dependence of polarization [Li et al., *J. Am. Chem. Soc.* 140, 2214 (2018)], respectively, in each of three emerging thin-film ferroelectric materials: indium selenide (a-In₂Se₃), nanometer barium titanate (BaTiO₃) films on Ge(001), and calcium-manganese titanate alloys (Ca_{2-x}Mn_xTi₂O₆). By probing ferroelectricity in real time, SHG helps optimize film growth conditions (e.g. interfacial strain, chemical precursor composition) and develop molecular dynamic and first-principles structural models of ferroelectric polarization. Finally, in collaboration with B. Korgel (UT Chem. Eng.), we measured absolute two-photon absorption (2PA) cross-sections of ligand-passivated, nanometer-diameter silicon nanocrystals in aqueous suspension, and demonstrated 2PA confocal microscopy of mouse cells incubated with the non-toxic nanocrystals [Furey et al., *phys. stat. sol. (b)* 255, 1700501 (2018)].

MICHAEL P. DOYLE, AX-1871, The University of Texas at San Antonio. SELECTIVE CHEMICAL OXIDATIONS.

We have completed research directed to the conversion of enol ethers and enamides to unsaturated carbonyl compounds, developed the oxidative replacement of dinitrogen in diazocarbonyl compounds by oxygen transfer from 2,6-dichloropyridine-N-oxide, and undertaken new peroxide addition reactions that show high promise for broad applications. The oxidative procedure used for diketooesters has shown remarkable reactivity and selectivity in asymmetric ene reactions and aldol condensation reactions and will be used to elaborate other condensation reactions; these reactions occur at room temperature, and the pyridine product does not coordinate with dirhodium(II) to inhibit catalysis. The focus of most of our efforts during the past few months has been the tert-butyl hydroperoxide/chloroform reaction with styrenes that involves the regiospecific addition of the dichloromethyl radical and tert-butylperoxy radical to styrene and substituted styrenes in very high yield. This transformation is effectively catalyzed by dirhodium caprolactamate or cuprous iodide at room temperature, requires a tertiary aliphatic amine to form the dichloromethyl radical, and appears to be general for haloform reactions. The mechanism of this reaction is complex and appears to be governed by factors that have not been previously considered. Of fundamental importance is the question of how haloforms can be either a hydrogen atom donor or a halogen atom donor. Efforts are also underway to develop the same reaction for the addition of dihalomethyl and hydroxyl, as well as to broaden the scope of the alkenes that can be used. Detailed investigations of the catalytic reactions of styrenes with tert-butyl hydroperoxide in the absence of haloform and amine have revealed the formation of their 1,2-di-tert-butyl peroxide derivatives, as well as several mono-peroxides in lower yields, and, eventually, products from C=C bond cleavage in high yield. Addition precedes C-C bond cleavage.

RUI-RUI DU, C-1682, Rice University. INFRARED AND MICROWAVE SPECTROSCOPY OF ATOMICALLY LAYERED MATERIALS.

Microwave Photocurrent from the Edge States of InAs/ GaSb and InAs/InGaSb Bilayers

We measure microwave photocurrent in devices made by InAs/GaSb and InAs/InGaSb bilayers, where both insulating bulk state and conducting edge state were observed in the inverted-band regime, consistent with the theoretical prediction for a quantum spin Hall (QSH) insulator. It has been theoretically proposed that microwave photocurrent could be a unique probe in studying the properties of QSH edge states. To distinguish possible photoresponse between the bulk state and the edge state, we prepare two types of samples, i.e., Hall bar and Corbino disk, from the same wafer. A back gate is used to tune Fermi level into the bulk gap. Results show that the Corbino disk samples have a negligible photocurrent in the bulk gap. On the contrary we observe clear photocurrent signals from the Hall bar samples in the bulk gap. This finding suggests that the photocurrent may carry information concerning the electronic properties of the edge states. We have studied the frequency, temperature, and magnetic field dependence of the photocurrent.

Quantum Quasiparticle Interference on the surface of Weyl Semimetal by Scanning Tunneling Microscopy

We have imaged the atomic structure and quantum quasiparticle interference (QPI) on the surface of Weyl semimetal (TaAs) using a low temperature scanning tunneling microscopy/spectroscopy equipped with vector magnets. The sample surface that is being studied is prepared by UHV in situ cleavage. Ta- and As- terminated surfaces are observed with atomic scale. QPI patterns that arise from quasiparticle scattering of the surface states including the topological Fermi arcs in TaAs are observed on As- and Ta- terminated surfaces respectively and compared without/with external magnetic field. The electron scattering near the atomic steps are also investigated. The results should help us to understand the electron scattering behaviors of the topological Fermi arcs.

KIM R. DUNBAR, A-1449, Texas A&M University. MAGNETIC AND ELECTRONIC PROPERTIES OF MOLECULAR MATERIALS.

The overarching theme of this project was to study the magnetic properties of small molecules with specific geometries and electronic configurations in order to understand the fundamental underpinnings of how structure and electronic properties dictate anisotropy and how they affect the mechanism(s) involved in slow paramagnetic relaxation of Single Molecule Magnets (SMMs). In the last funding period, our modular approach to designing homologous series of compounds led to families of compounds with the same geometrical arrangement of spin centers. Using theory as our guide, we advanced fundamental knowledge regarding how single-ion anisotropy in specifically targeted mononuclear geometries, viz., linear, trigonal planar, mono-

pyramidal, and trigonal bipyramidal affects zero-field splitting and, hence magnetic bistability. Despite the few number of spins that they possess, such molecules are excellent prospects for SMMs.

An additional geometry that we are exploring especially is the pentagonal bipyramid, a coordination number that had been a topic of investigation in our laboratories for several years before the discovery that molecules exhibiting this structural type are excellent SMMs. We verified a theory that the heptacyanomolybdate(III) anion is an excellent prospect for creating a barrier to reversal of the magnetization in trinuclear complexes with spin centers coordinated in the axial positions of the pentagonal bipyramid. The complex holds the record for the highest temperature barrier and hysteresis for cyanide SMMs. We have expanded on this subject by designing new molecules of both d block and f block elements with ligands that enforce rigid pentagonal bipyramidal geometry.

This research has been an excellent platform for training students and post-graduates in interdisciplinary research and is an effective tool for the development of excellent problem solving skills in a highly collaborative environment.

F. BARRY DUNNING, C-0734, Rice University. STUDIES INVOLVING MOLECULES IN HIGH RYDBERG STATES.

Cold 84Sr atoms held in a dipole trap have been used to examine the formation and properties of ultralong-range Rydberg molecules in which scattering of the excited electron in a Rydberg atom from one, or more, neighboring ground-state atoms creates a novel chemical bond. The formation of dimers, trimer, tetramers, . . . has been explored. Measurements have been extended to high density samples (Bose-Einstein condensates (BECs)) to create molecules having tens to hundreds of ground-state atoms within the electron orbit. This has allowed spectroscopic observation of a collective response and formation of quasi-particles known as polarons consisting of the Rydberg "impurity" dressed by excitations of the background medium. The mechanism leading to the destruction of Rydberg molecules in a dense BEC have also been elucidated and can be explained using a model that emphasizes the interaction between the Rydberg core ion and nearest-neighbor ground-state atom. Measurements are being extended to study the effects of quantum statistics, which affect the pair correlation function of $g(2)(R)$, on molecule formation. These measurements are being undertaken using (fermionic) 87Sr . Since 87Sr has a sizable nuclear spin ($I=9/2$) its excitation spectrum is complicated by hyperfine interactions which required a detailed study of its excitation spectrum to identify the states of interest. Preliminary work using a polarized 87Sr sample have shown that, at temperatures where quantum statistics become important and reduce $g(2)(R)$, dimer and trimer production are substantially reduced. In other work using a hot atomic beam the cross sections for Rydberg atom loss through Rydberg-Rydberg collisions are being examined. The cross sections are large and are well-described by a hard-sphere collision model.

The autoionization of very-high- n Rydberg states was also studied as a prelude to creation of long-lived two-electron-excited "planetary atom" states in strontium.

RON ELBER, F-1896, The University of Texas at Austin. BRIDGING TEMPORAL AND SPATIAL SCALES IN MEMBRANE MODELING.

Our research project is on multi-scale modeling approaches with a focus on membranes. In the last year, we have made considerable progress in both, further development of computational approaches and in concrete investigations of membrane properties. In the recent manuscript of Fathizadeh and Elber, we addressed the problem of simulating heterogeneous membranes. Biological membranes are extremely complex systems that consist of thousands of types of lipid, sterols and protein molecules. As such they present a profound challenge for computer simulations. For example, as the number of components increases the number of phases increases as well. In biology, rafts, which are patches with different composition of phospholipids and sterols embedded in the membrane, were proposed to support protein insertion and hence have a specific biological function. Proving the existence and functions of rafts in biological systems remained challenging from both, computational and experimental perspectives. To investigate the thermodynamically stable state of extremely heterogeneous membrane we introduced the algorithm of MDAS (Molecular Dynamics with Alchemical Steps). It is a combination of conventional MD (Molecular Dynamics) and non-equilibrium trajectories to estimate the statistical weight of configurations. We have shown that rapid equilibration in the mixture of DOPC and DPPC lipids is obtained using MDAS, equilibration that is much hard to achieve with conventional MD. The speedup factor is estimated to be in the thousands, which opens the way for a new class of studies. In another paper, we investigated the impact of counter ions on the structure and dynamics of heterogeneous and negatively charged membranes (a mixture of PC and PS). This study was conducted in collaboration with the experimental group of Carlos Baiz from UT chemistry that use 2D IR to study membrane properties. We identify binding sites of calcium at the membrane interfaces.

ANDREW D. ELLINGTON, F-1654, The University of Texas at Austin. KINETIC AND STRUCTURAL CHARACTERIZATION OF THE FIRST ERROR-CORRECTING REVERSE TRANSCRIPTASE.

Our previous work on RTX (published in Science) expanded the template specificity of KOD polymerase to utilize RNA ($2' - \text{OH}$), in addition to native DNA ($2' - \text{H}$). We have now expanded the substrate specificity to include $2'$ -O-methyl (2Ome) templates. Some 18 rounds of directed evolution identified some two dozen mutations that increased the polymerase's ability to utilize non-standard templates, and testing of individual polymerase variants led to enzymes that could broadly utilize DNA, RNA, and 2Ome nucleic acids as templates during replication. In consequence, we are now able to efficiently reverse transcribe a 50 nucleotide template containing solely 2Ome residues, and amplify RNA templates over 5 kilobases in length. The resultant enzyme is also capable of proofreading on DNA, RNA, and 2Ome templates. These novel findings demonstrate that error correction is compatible with non-standard templates, even when the enzyme is a generalist. In the next iteration of Welch funding, we will use these evolved enzymes to further explore the mechanistic relationship between template recognition and proofreading.

A potential novel application of high-fidelity XNA reverse transcriptases is for digital information storage, since evolved polymerases uniquely enable XNAs to be read by next-gen DNA sequencing technologies. Using chip-based XNA synthesis we encoded a series of digital files into both standard

DNA and 2Ome oligonucleotide sets, and are now determining whether this encoded information can be efficiently read by the evolved polymerase. We propose that the 2Ome polymerase could be an efficient proof of concept in demonstrating the new field of 'cryptogenetics.' The cryptogenetic technology presents a novel platform for digital information security that is unique in that it leverages atomic scale specificity of enzymes instead of digital keys. We envision that this technology may be particularly useful for privileged information such as secure archival storage.

JAN P. ERZBERGER, I-1897, The University of Texas Southwestern Medical Center. STRUCTURAL AND BIOCHEMICAL CHARACTERIZATION OF DEAD-BOX ATPase FUNCTION AND REGULATION DURING RIBOSOME BIOGENESIS.

Over the past year, we have incrementally optimized our overexpression and purification system to maximize intermediate yield and reduce non-specific interactions during purification. This is an essential process to ensure that we are capturing transient, highly dynamic assemblies. These optimized strains, harboring a STREP-tag, can now be purified rapidly and with minimal background. Importantly, our samples reveal protein banding patterns that are different from those obtained when ribosomal intermediates are purified using overexpressed, affinity-tagged wild-type protein. We have also optimized our cryo-EM grid preparations using quantifoil grids with a layer of continuous carbon and are currently collecting data on our first set of intermediates. Additionally, our purified samples are being analyzed by cross-linking mass spectrometry (XL-MS). We anticipate that we will have our first single-particle reconstructions within the next month.

In parallel to these efforts, we have continued to characterize the interactions between DEAD-box proteins and factors identified in our XL-MS screens. One such interaction, between the DEAD-box protein Drs1 and the biogenesis factor Nop12 has revealed Nop12 to be a modulator of the ATPase activity of Drs1. Using truncations, we find that activation is dependent on the C-terminal extension of Drs1. Additionally, Nop12 stimulates Drs1 only in the presence of yeast total RNA, but not polyA RNA, suggesting that Nop12 may stimulate the functional interaction between Drs1 and the type of complex RNA structures found in ribosomal RNA (the main component of yeast total RNA). These studies will also reveal which RNA substrate is most suitable for X-ray crystallographic studies of the Drs1/Nop12/RNA complex.

In summary, our yeast strains are providing us with unique intermediates for structural and XL-MS analysis and our hybrid approach has allowed us to identify Nop12 as a modulator of Drs1 activity during 60S biogenesis.

DONGLEI L. FAN, F-1734, The University of Texas at Austin. INNOVATIVE MECHANISM FOR THE SYNTHESIS OF 3-D NANO-SUPERSTRUCTURES BY DESIGNED CATALYSTS.

In this grant year, we made substantial progresses in two aspects:

(1). We investigated an innovative approach to synthesize 3D ramified porous graphite foams (RPGFs) by strategically creating 3D catalytic foams with hierarchical and diverging microscale branches and pores. This work can readily address the "double low" issue of the energy-storage supercapacitors. The fabrication strategy and the obtained materials are reported for the first time. Arrays of graphitic microtubes (2-5 μm in width, $\sim 30 \mu\text{m}$ in length) covalently grown on porous graphite can be obtained with high uniformity and reproducibility. They fully fill in the large interspace of $\sim 100\text{-}200 \mu\text{m}$ between graphitic struts of conventional 3D GFs, which readily boosts the volumetric surface area by three times and enables a doubled loading of pseudocapacitive materials (Mn_3O_4 , 3.91 mg cm^{-2} , 2.78 wt%), compared to those of conventional GFs. Further experimental characterization shows that the half RPGF/ Mn_3O_4 (RPGM) composite electrodes offer an areal capacitance as high as 820 mF/cm^2 (1 mV/s) without utilization of binders or conductive additives. They also retain 88% capacitance and 98% coulombic efficiency after 3,000 charging/discharging cycles at 20 mA/cm^2 . When assembled into all- solid-state symmetric supercapacitors, the full-cell capacitance reaches 191 mF/cm^2 (2 mV/s). Moreover, owing to the porous structures, the full supercapacitors are highly flexible and maintain 80% capacitance after 1,000 bending cycles, outperforming most manganese oxide/GF supercapacitors. Finally, we applied the energy devices to directly integrate and power a nanomotor manipulation system.

(2) We initiated and explored a new concept of additive synthesis of 3-D functional porous composites based on chemical assembly. We demonstrated the concept in a preliminary study of a 3-D porous polymer composite foam coated with MoS_2 /carbon microbeads for applications in solar steaming.

LEI FANG, A-1898, Texas A&M University. PI-CONJUGATED MACROCYCLIC MOLECULAR BELTS.

Thermodynamically controlled RCM is a powerful tool to construct a fully conjugated ladder-type structure from a vinyl-functionalized conjugated precursor. We envisioned that this strategy has great potential to synthesize cMMB, a class of linear analogues of cMMB – benzo[k]tetraphene-derived fused-ring hydrocarbons (BTp) with up to 13 fused rings – were successfully synthesized. Furthermore, comprehensive analysis of ladder-type BTp oligomers was accomplished to afford their optical properties, effective conjugation length, and solid-state dynamics. This efficient method also allowed to synthesize various carbazole and indolo[3,2-b]carbazole-based ladder-type heteroarenes with up to 11 fused rings, which showed structural planarization-induced charge transfer complex formation with electron deficient F4TCNQ. Another strategy we investigated for the construction of ladder-type structure is to employ intramolecular non-covalent bonds to lock the coplanar conformation. In order to overcome the poor solubility of the rigid coplanar polymer, A well-solubilized, non-coplanar polymer precursor with thermally cleavable Boc groups (hydrogen bond inhibitor) was synthesized and processed into thin films. After in situ removal of Boc groups upon thermal treatment, the regenerated latent intramolecular hydrogen bonds led to the rigid ladder-type conformation. In addition, we studied and developed a number of macrocyclization reactions potentially useful for cMMB synthesis. A scalable, cost-effective aldol triple condensation reaction was discovered serendipitously during the exploration, leading to efficient synthesis of conjugated PPNs. The resulting PPNs prepared from inexpensive starting

materials exhibited rapid and selective adsorption of organic molecules in aqueous environment suggesting the function of size-specific macrocyclic cavities in the polymer.

WALTER L. FAST, F-1572, The University of Texas at Austin. **CHEMICAL PROBES FOR BIOLOGICAL CATALYSTS.**

We report on work in eight papers (in press or published) during this period: Two papers (last reported as submitted) were revised and published, and describe use of a fragment-based approach to develop dipicolinic acid derivatives as nanomolar inhibitors of dinuclear zinc metallo-beta-lactamases, and our analysis of how clinical mutants impact metal ion and ligand affinity. An additional publication elucidates the mechanism of inhibition by aspergillomarasmine A. We made a wider comparison of inhibition mechanisms for metallo-beta-lactamases in a review article. Use of spectroscopy and other methods distinguished inhibitors with metal-stripping mechanisms from those that form stable ternary complexes, an important difference in development of selective probes that is often overlooked for this target. We were the first group to discover some clinical variants have evolved to overcome zinc scarcity. In a paper recently accepted (J Biol Chem), we extended these studies using a wider panel of clinical mutants to reveal the evolution of increased zinc affinity and the ability to function effectively as monozinc catalysts. In other ongoing work, we continued development of covalent probes, optimizing target selectivity for 4-halopyridine enzyme inactivators. We “dissected” a 2-chloroamidine-based inactivator and analyzed the fragments separately to aid probe optimization in a paper recently accepted (Biochemistry). Finally, an invited “Perspectives” article was used to advocate use of a mechanistic taxonomy for classifying covalent inhibitors to better describe the varied mechanisms used to achieve target selectivity. In sum, development of chemical probes to study biological catalysts continues to be a fruitful area of study and will continue in the following grant period.

SHERVIN FATEHI, BX-1921, The University of Texas Rio Grande Valley. **STOCHASTIC METHODS FOR HIGHLY ACCURATE QUANTUM CHEMISTRY EXTENDED TO NONADIABATIC MOLECULAR DYNAMICS.**

For the first budget period, my goal was to recruit a postdoctoral fellow and an undergraduate student to implement dynamical calculations using stochastic electronic-structure methods. These goals were premised on Spring 2017 completion of a server room for my high-performance computer (HPC). Renovations were plagued by material & work delays and failures of the electricians to perform work consistent with vendor specifications; construction was only finished in late May 2018. I had quotes ready for the budgeted Permanent Equipment, however, and it was purchased and installed within a month. Thanks to the Foundation, we obtained additional solid-state hard drives (480 GB capacity) for each compute node of the HPC system and upgraded the internal networking switch.

Without all HPC resources in place, recruiting a capable postdoctoral fellow has been challenging. Still, I interviewed candidates from Texas Tech and from the University of North Texas. Full-scale recruitment will continue on community lists and job boards. In the interim, my undergraduate student Catherine Clark has been adding driven molecular dynamics methods into the Q-Chem codebase and interfacing external programs with it. I am actively seeking another talented undergraduate student to work on this research full-time.

Using Travel funds, I attended the Welch Conference and the ACS Southwest Regional Meeting, where I gave a talk, “Toward a complete framework for nonadiabatic dynamics (with full configuration interaction).” I examined aspects of my previous work aligned with this project, as well as its theoretical basis—our insight that nuclear forces can be determined for converged stochastic wavefunctions without response calculations. During the second budget period, I will move quickly to complete hiring, and to press forward with highly accurate dynamics simulations so that we can present and publish new results as soon as possible. Thank you for your continuing support!

MICHAEL FINDLATER, D-1807, Texas Tech University. **BASE-METAL CATALYZED TRANSFORMATIONS.**

The first year of the grant period saw significant progress in a number of areas related to the exploration of new transformations. This year we focused primarily on hydroboration catalyzed by first-row metal elements, with exciting discoveries in iron, cobalt and nickel chemistry.

With the generous support of the Welch Foundation, we have developed a nickel-catalyzed and regioselective hydroboration of N-heteroarenes - such transformations are typically carried out using expensive precious metals; a nickel-catalyzed process is unreported in the literature. This work for recently accepted for publication (ACS Catalysis). Our work with iron based catalysts (described in last year's progress report) was published this year (J Org Chem) and prompted us to study related cobalt chemistry. The chemical reduction of carbon dioxide (CO₂) has the potential to turn a potent greenhouse gas into a new C1 feedstock for the chemical industry, with this in mind we studied the cobalt-catalyzed reduction of CO₂ using a hydroboration strategy. Our results were recently published (Dalton Trans) and were only the second literature report on CO₂ hydroboration using cobalt. We plan to explore this chemistry further by: 1) studying the reaction mechanism with the goal being design of a superior catalyst and, 2) using this strategy to incorporate CO₂ into organic substrates to generate value added organic molecules.

Finally, thanks to the support of the Welch Foundation, our publication in the field of ATRA (Atom Transfer Radical Addition; last year's progress report) has led to collaboration with the groups of Marks and Stoddart at Northwestern on expansion of this chemistry to a range of new metal complexes and catalysis which was recently submitted for publication (Inorganic Chemistry). We believe this collaboration will provide the foundation for future publications and research grant applications in the areas of synthesis and catalysis.

ILYA J. FINKELSTEIN, F-1808, The University of Texas at Austin. MAPPING THE PROOFREADING MECHANISMS OF Cas9 NUCLEASE ON A HACKED DNA SEQUENCER.

In the last funding period, we repurposed next-generation sequencing chips to simultaneously measure the interactions between proteins and $\sim 10^7$ unique DNA sequences. We next used this platform (called CHAMP) to comprehensively profile off-target DNA binding of a Type I-E CRISPR/cas complex. Using this rich dataset, we next determined biophysical models to explain off-target DNA binding in that system. This work was published in Cell.

In the last year, we have expanded this platform to profile new and emerging CRISPR nucleases, including natural Cas9 and engineered variants that report to have a higher fidelity. We also began to biophysically characterize Cas12a (Cpf1), a recently-discovered RNA-guided nuclease that is purported to have a higher fidelity than Cas9. Our first paper on Cas12a was recently published in Molecular Cell. Two additional manuscripts on Cas9 and Cas12a are also in preparation. We also developed a new method, called NucleaSeq, for measuring DNA cleavage of all likely off-target DNA molecules. We developed this because CHAMP only reports on protein-DNA binding but not DNA cleavage. For NucleaSeq, a synthetic library containing a set of on-target and off-target DNA sequences is incubated with Cas9 (or any other nuclease) for increasing amounts of time. The DNA from each time point is submitted for deep sequencing. This data is most comprehensive comparison of engineered Cas9 variants. For example, we find that even high-fidelity variants bind off-target DNA as avidly as the wt Cas9 but only one engineered Cas9 reduces off-target DNA cleavage. In contrast, wild type Cas12a shows both high fidelity DNA binding and cleavage, possibly supplanting Cas9 as the go-to tool for precision genome editing.

Finally, the Welch Foundation has enabled new exciting research areas in my lab. Briefly, these include new tools for mapping epigenetic inheritance in single cells and single-molecule biophysical studies of emerging CRISPR systems.

PAUL F. FITZPATRICK, AQ-1245, The University of Texas Health Science Center at San Antonio. MECHANISMS OF ENZYMES.

We have continued studies of I366N tryptophan hydroxylase, a non-heme iron enzyme. This mutation of a key residue in a mobile active-site loop decreases by 2000-fold the rate constant for formation of the initial intermediate with oxygen without altering subsequent steps. By analyzing the effects of changing the solvent viscosity on the kinetics, we have shown that the effect of the mutation can be assigned to a change in the dynamics of the active site loop. This establishes that closure of this loop over the active site is coupled to the first step in catalysis. We have also examined the effect of phosphorylation of phenylalanine hydroxylase on its activity and allosteric properties. Stopped-flow studies of the kinetics of the conformational change that occurs upon binding of phenylalanine to the allosteric site are consistent with a model in which a slow conformational change to a more active form is followed by equilibrium binding of two molecules of phenylalanine to the dimeric regulatory domain. Phosphorylation of Ser16 alters the equilibrium constant between the low activity form and the activated form 10-fold by increasing the rate constant for the conformational change to the active form without affecting the intrinsic affinity for phenylalanine. This results in the phosphorylated enzyme becoming activated at lower concentrations of phenylalanine. There is no effect of phosphorylation on the catalytic activity of the activated form.

SKYE FORTIER, AH-1922, The University of Texas at El Paso. NEW VISTAS IN EARLY ACTINIDE CHEMISTRY.

We have been studying the structure and reactivity of the uranium(III) complex LUI(DME) ($L = [\text{bis}(2,6\text{-iisopropylanilide})\text{terphenyl}]_2$ -) which has proven to be an amenable platform for synthetic elaboration.

For instance, addition of the metalloanion $[\text{Na}(\text{tmeda})][(\text{Cp})\text{Fe}(\text{CO})_2]$ to LUI(DME) produces the heterobimetallic complex $\text{LU}[(\text{Cp})\text{Fe}(\text{CO})_2]$ which features the first structurally characterized, unsupported U-Fe bond. The electronic structures of both LUI(DME) and $\text{LU}[(\text{Cp})\text{Fe}(\text{CO})_2]$ were investigated at a high level of theory in collaboration with Dr. Bess Vlaisavljevich of USD. Interestingly, despite the coordination of soft donors to uranium, covalency in the U-arene and U-Fe bond are minimal. However, electrochemical and computational analyses indicate novel redox chemistry that may afford unusually reduced compounds. These results were recently reported in Organometallics. Endeavors are underway to synthesize the Ru and Os analogs to study group bonding trends. In addition to this, the magnetic properties of LUI(DME) are currently being examined by SQUID magnetometry. Preliminary experiments show that reactions with LUI(DME) and the group 6 metalloanions $\text{Na}[(\text{Cp})\text{M}(\text{CO})_3]$ ($M = \text{Mo}, \text{W}$) appear to give new heterobimetallic compounds which are currently being characterized.

In relation to this work, Welch funding also supported the authoring of a comprehensive book chapter on the chemistry of pentavalent uranium, and this chapter is currently in press.

As an extension of this uranium-arene project, we have also looked at the coordination chemistry of the $[\text{bis}(2,6\text{-iisopropylanilide})\text{terphenyl}]_2$ -ligand with Dy(III). The architectural features of the bis(anilide) terphenyl ligand may be useful for accessing single molecule magnets with exceptional magnetic properties. The dysprosate complex $[\text{K}(\text{DME})_3][\text{LDy}(\text{Cl})_2]$ has been synthesized and the compound is presently under magnetic study by our collaborator Dr. Muralee Murugesu of the University of Ottawa.

MATTHEW S. FOSTER, C-1809, Rice University. QUANTUM COHERENCE IN DRIVEN, DISORDERED AND TOPOLOGICAL MANY-BODY SYSTEMS.

We published three papers this year, including two in Physical Review Letters. The Letters represent key achievements in my research group in the past several years. In one of them (Liao 2018), we pioneered a new approach towards understanding the many-body localization (MBL) transition in a system of interacting fermions, with quenched disorder. We considered a system with short-ranged interactions, appropriate to an ultracold atomic Fermi gas experiment. Our approach involves an expansion on the metallic side, where we demonstrated that the dephasing of quantum interference that leads to classical transport on the largest scales is more complex for such a system than originally thought. Dephasing occurs due to the random thermal fluctuations of the gas,

which spoil the delicate interference responsible for Anderson localization. In this case, we noted that these fluctuations are strongly non-Markovian, and this means that the “bath” dephases less efficiently than expected at low temperatures. Using a novel expansion, we identified a phase transition corresponding to the deconfinement of a self-interacting polymer loop, and associated this to the failure of dephasing. This could signal a transition into the MBL phase. With the same student, we also published a long paper in *Annals of Physics* detailing the encompassing formalism leading to the problem posed in the Letter.

In our second Letter (Ghorashi 2018), we showed that contrary to expectations most surface states of bulk topological superconductors show robust criticality in the presence of quenched disorder (impurities). In particular, we found that almost every surface state exhibits statistics consistent with classical critical percolation (in two dimensions). Since the latter is equivalent to a certain type of quantum Hall plateau transition, we have demonstrated the remarkable fact that surface states of topological superconductors consist largely of “stacks” of critical plateau transition states.

KENDRA K. FREDERICK, I-1923, The University of Texas Southwestern Medical Center. **PROTEIN-MEDIATED TRANS SPLICING FOR POLYMORPHIC AMYLOID STRUCTURE DETERMINATION.**

My research goal is to understand how biological environments influence protein structure. We focus on how cellular environments restructure proteins that are metastable, contain intrinsically disordered domains, or both. To pioneer the application of sensitivity-enhanced DNP NMR we study a system with highly tractable genetics, the yeast prion protein Sup35. This protein can adopt a self-templating amyloid fold that is stably inherited from mother to daughter cells and changes the cellular phenotype. This protein-based mechanism of inheritance requires the action of molecular chaperones. The intrinsically disordered region of Sup35 that flanks the amyloid in purified samples is restructured when Sup35 is templated in cellular environments. We are using protein chemistry approaches to isotopically label small regions with the goal of obtaining atomic resolution structural information. We are also making mutant yeasts with perturbed chaperone environments with the goal of determining if and how different chaperones alter Sup35 structure.

The Welch Foundation supports the training of a post-doctoral scholar with expertise in magic angle spinning solid state NMR, Yiling Xiao. In my group, she is complementing her training in spectroscopy with a specialization in DNP, which has included external training at the National High Magnetic Field Laboratory in Tallahassee and at the Winter School for Biomolecular Solid State NMR. Yiling’s principle interest is to determine the arrangement of monomers in Sup35 fibers. She is second author on a manuscript that was submitted to *Methods in Enzymology* and has two articles in preparation.

Support from the Welch Foundation supported training of NSF Graduate Research Fellow, Whitney Costello. Whitney’s principle interest is to develop in-cell NMR techniques and she is first author on a manuscript submitted to *Methods in Enzymology* and has another article in preparation.

BENNY D. FREEMAN, F-1924, The University of Texas at Austin. **SYNTHESIS AND CHARACTERIZATION OF WATER AND ION TRANSPORT IN NOVEL ION EXCHANGE MEMBRANE POLYMERS.**

We recently developed a theoretical framework to permit calculation of fundamental ion transport properties in charged polymers (ion exchange membranes (IEMs)), which is important in membranes for water purification, batteries, and renewable energy generation. We validated this framework via careful, systematic measurements of water and ion sorption, permeability, and ionic conductivity (Macromolecules, DOI: 10.1021/acs.macromol.8b00645). We are extending this framework to Nafion, the benchmark IEM used in fuel cells. Nafion has a significantly different chemical structure and morphology than previous IEMs studied. Preliminary results for NaCl and MgCl₂ sorption in Nafion show that the model describes the experimental data remarkably well. Concurrently, we are developing previously unexplored routes to synthesize and characterize highly selective and permeable IEMs with superior mechanical properties. Current IEMs are brittle, crosslinked polyelectrolytes that require thick support structures for sufficient mechanical stability which then reduces their throughput. Using concepts from the biomedical field, where super-tough polymers have been synthesized for cartilage replacement, we developed prototype “super-tough” IEMs. We are optimizing synthetic procedures to reduce water content, enhancing selectivity for membrane applications. We also published an article reporting a rapid, accurate method to measure ionic conductivity in IEMs (*J. Membrane Sci.*, DOI: 10.1016/j.memsci.2017.10.024). This article resolved longstanding inconsistencies in such measurements in the literature, providing a new, reliable technique for such studies. These results on the modeling, synthesis and characterization fronts this year provide a solid foundation to perform exciting and important studies during the coming year.

FRANÇOIS P. GABBAÏ, A-1423, Texas A&M University. **TUNING THE ELECTROPHILIC PROPERTIES OF GROUP 10 METAL COMPLEXES USING NON-INNOCENT ANTIMONY Z-LIGANDS.**

As part of our continuing investigations of the multifaceted properties of antimony ligands, we have continued to target transition metal complexes in which the catalytic properties of the metal center can be controlled by the chemistry taking place at the antimony atom. In one of our most important achievements dealing with complexes featuring a Pt->Sb bond, we have found that fluoride anion abstraction from the antimony atom provides an effective means for increasing the electrophilic character of the platinum center. This conclusion was derived from an exhaustive characterization of the complexes involved, a computational investigation of their electronic structure and their catalytic properties. In a related effort, we have investigated Pt-Sb complexes in which an antimony-substituted bipyridine ligand is coordinated to platinum. In this case, we found that oxidation of the antimony center could be used to influence the electrophilic character of the antimony center. These results underscore the functional versatility displayed by antimony ligands, the chemistry of which can be manipulated to enhance catalysis at a nearby transition metal site. We have obtained corroborating results in the chemistry of T-shaped gold-stiborane complexes in which the electrophilic character of the gold center is enhanced by the presence of an Au->Sb interaction. This enhancement becomes manifest in the carbophilic properties of the gold center and its ability to mediate reactions necessitating alkyne activation. Our work on complexes featuring a Lewis acidic antimony moiety in the secondary coordination sphere of transition metals has served as an inspiration for the study of gold complexes featuring a

dangling H-bond donor group which helps activate the gold center by chloride anion abstraction. Finally, this grant has continued to support our fundamental investigations into the chemistry of main group Lewis acids and their ability to activate small molecules or bind anions.

ELYSSIA S. GALLAGHER, AA-1899, Baylor University. CAN WE APPLY HYDROGEN/DEUTERIUM EXCHANGE – MASS SPECTROMETRY TO ELUCIDATE GLYCAN BINDING INTERACTIONS?

In-ESI HDX-MS experiments involved analyzing the effects of source parameters and sample conditions on HDX of carbohydrates to identify a set of conditions to use in further analyses. As part of this work, we monitored differences in carbohydrate conformations by in-ESI HDX using different solvents. With molecular modeling, we were able to assign these structural differences to changes in the intra- and inter- molecular hydrogen bonding within a model carbohydrate. This work has been submitted for publication. A benefit of in-ESI HDX is its ease of implementation. Yet, the magnitude of HDX measured on different days varied, likely due to changes in ambient humidity in the ESI source. We developed an internal standard by derivatizing maltoheptaose with Girard's T reagent. When the internal standard was used for in-ESI HDX, the relative HDX was more repeatable on different days. This experimental work is complete, and a manuscript is in preparation.

We performed HDX experiments using theta tips. Our current data shows that theta tips can be used to label carbohydrate hydroxyls by HDX and the extent of labeling can be altered by modifying the tip size. A manuscript for this work is in preparation.

Rapid HDX methods can be used to distinguish differences in carbohydrate structure. Using our internal standard, we were able to distinguish differences in HDX for two trisaccharide structural isomers using in-ESI HDX. We also observed differences in the relative HDX for tetrasaccharides and pentasaccharides adducted to different metal ions. This data illustrates that in-ESI HDX can also distinguish structural differences associated with adduct formation.

These results were presented at six meetings in 2017 and 2018, including the 65th and 66th ASMS Conferences on Mass Spectrometry and Allied Topics, the Gordon Research Conference on Carbohydrates, SCIX2017, the American Chemical Society Southwest Regional Meeting, and the TX Enzyme Mechanisms Conference.

VENKAT GANESAN, F-1599, The University of Texas at Austin. FUNDAMENTAL STUDIES OF SELF-ASSEMBLY IN MIXTURES OF ORGANIC AND INORGANIC MOLECULES.

We used atomistic molecular dynamics simulations to study ion mobilities and the molecular mechanisms of transport in blends of poly(1-butyl-3-vinylimidazolium-hexafluorophosphate) electrolytes with 1-butyl-3-methylimidazolium hexafluorophosphate ionic liquids. We characterized the structural and dynamical properties of the blend electrolyte systems through radial distribution functions, diffusivities, conductivities, different time scales of relaxation, and probed the correlations underlying such characteristics. Our results indicate that many features of ion transport in such blend systems mirror those observed in our earlier study on pure polymerized ionic liquids. Explicitly, we observe that the anions associated with the polymerized cation move along the polymer backbone via the formation and breakup of ion-pairs involving polymerized cationic monomers of different polymer chains. However, as a result of the influence of mobile cations, an optimal blending composition achieves the highest conductivities at a temperature normalized by the glass transition temperature. These results provide new insights into the mechanism of ion transport in multicomponent ionic liquid systems.

In a recent study, by using atomistic computer simulations on a series of experimentally studied polymers, we demonstrated a monotonic correlation between ion conductivities and the respective dielectric constants of the electrolytes. In the present study, we use coarse-grained molecular dynamics simulations to demonstrate that such a monotonic correlation does not persist indefinitely, and instead, as a consequence of the competition between ionic aggregation and polymer segmental dynamics, ionic conductivity maximizes at an intermediate polymer polarity dipole moment strength. Such results shed light on the limits to which polymer dielectric constant can be used to influence the ionic conductivity of electrolytes.

ISAAC GARCIA-BOSCH, N-1900, Southern Methodist University. EFFICIENT, SUSTAINABLE, AND SELECTIVE CATALYTIC SYSTEMS FOR THE DIRECT C-N FUNCTIONALIZATION OF C-H AND C=C BONDS BASED ON IRON-NITRENOID/IMIDO SPECIES.

Metal complexes bearing redox-active ligands with tunable H-bonding groups.

A1) Synthesis and characterization of bidentate ligands containing H-bonds based on the 1,2-phenylenediamine (NHRPhN2H2) and ethylenediamine (NHREtN2H2). With these ligand scaffolds, we have been able to synthesize and characterize a series of Fe, Co, Ni, Cu and Zn complexes. X-Ray diffraction analysis showed that the geometry of the complexes was highly influenced by the ligand (both diamine backbone and H-bonding group) and metal used. We observed that the H-bonding groups interacted in an intramolecular fashion with the other ligand and the metal center. These H-bonding interactions are highly influenced by the ligand used and geometry of the complex; different R groups of the urea moiety lead to variations in the intramolecular H-bonding distances. To the best of our knowledge, this family of complexes (more than 20 X-ray structures) constitutes the first example of metal complexes in which the strength of the H-bonding interactions can be tuned.

A2) We studied the reactivity of the Cu complexes [(NHRPhN22-)2CuII]2+ in the catalytic dehydrogenation of C-H bonds. Interestingly, our complexes perform this transformation using O2 as oxidant and without the addition of additives (Cu-based catalysts usually require the use of base and/or nitroxyl co-catalyst). Mechanistic studies suggest that our copper catalysts perform this oxidation in an unprecedented fashion for galactose oxidase model systems. These studies include detailed kinetic analysis and DFT calculations, in collaboration with Marcel Swart (University of Girona).

A research article describing these results will be submitted to JACS (August 2018).

B) Funds have also supported a project based on the use of Cu to hydroxylate sp² and sp³ C-H bonds. These findings will be submitted to *Angew. Chem. Int. Ed.* (August 2018).

JOHN A. GLADYSZ, A-1656, Texas A&M University. WERNER COMPLEXES AS "ORGANOCATALYSTS".

When NMR spectra of chiral racemic organic molecules containing a Lewis basic functional group are recorded in the presence of air/water stable salts of the cobalt(III) trication [Co((S,S)-NH₂CHPhCHPhNH₂)₃]³⁺ (23⁺), separate signals are usually observed for the enantiomers (28 diverse examples, >12 functional groups). Several chiral molecules can be simultaneously analyzed, and enantiotopic groups in prochiral molecules differentiated (16 examples). Particularly effective are the mixed bis(halide)/tetraarylborate salts 23⁺ 2X-BArf⁻ (X = Cl, I; BArf = B(3,5-C₆H₃(CF₃)₂)₄), which are applied in CD₂Cl₂ or CDCl₃ at 1-100 mol% (avg 34 and 14 mol%). Job plots establish 1:1 binding for -23⁺ 2Cl-BArf⁻ and 1-phenylethyl acetate or 1-phenylethanol, and ca. 1:2 binding with DMSO (CD₂Cl₂). Selected binding constants are determined. The NH moieties of the C2 faces of the trication are believed to hydrogen bond to the Lewis basic functional groups, as seen in the crystal structure of a DMSO solvate of -23⁺ 3I⁻. These salts rank with the most broadly applicable chirality sensing agents discovered to date.

These involve "legacy objectives" from earlier periods. The red orange fluororous rhodium (I) complexes ClRh(P((CH₂)_mRfn)₃)₃ (m/n = 2-3/6-10; Rfn = (CF₂)_n-1CF₃) are essentially insoluble in organic solvents at 20 °C, but have measurable solubilities in dibutyl ether at 55-65 °C. Under these conditions, they are effective catalyst precursors for the hydrosilylation of cyclohexanone by PhMe₂SiH. Upon cooling, the catalyst rest states precipitate, giving colorless solutions of C₆H₁₁O₂SiPhMe₂. When this sequence is conducted in the presence of Teflon® tape, the catalysts precipitate onto the tape, but desorb when used in subsequent cycles; Gore-Tex® membrane can be similarly employed. Rate measurements show an induction period in the first cycle, excellent retention of activity in the second and third cycles, and significant activity loss in the fourth.

VISHAL M GOHIL, A-1810, Texas A&M University. PHOSPHOLIPID REQUIREMENTS FOR MITOCHONDRIAL STRUCTURE AND FUNCTION.

To understand the role of nonbilayer phospholipids in mitochondrial respiratory chain (MRC) supercomplex formation, we have developed an ethanolamine (Etn) supplementation strategy – a method by which we can increase the mitochondrial non-bilayer phospholipid, phosphatidylethanolamine (PE).

Using this strategy, we tested the hypothesis that elevating mitochondrial PE could compensate for the loss of cardiolipin (CL), another nonbilayer phospholipid of mitochondria and demonstrated that:

- 1) Etn supplementation rescues MRC defects by promoting supercomplex assembly in CL deficient yeast cells.
- 2) Etn-mediated rescue occurs independently of its incorporation into PE. The rescue was specifically dependent on Etn, and not other phospholipid precursors such as choline or serine.
- 3) Etn analogues, including propanolamine are able to rescue the respiratory growth defect of CL- deficient yeast cells, but methylation of amine nitrogen of Etn abolishes the rescue.
- 4) Etn promoted supercomplex assembly in CL deficient cells by increasing the expression of MRC subunits.

These findings are published in *Journal of Biological Chemistry* (Basu Ball et. al., 2018, JBC).

We have also published a review titled "The role of nonbilayer phospholipids in mitochondrial structure and function" (Basu Ball et. al., 2018, FEBS Lett).

To determine the specific phospholipid requirements of MCU we have used yeast phospholipid mutants as surrogate systems to express the human and *D. discoideum* MCU and have found that:

- 1) CL is required for the abundance and activity of human and *Dd* MCU.
- 2) We also demonstrate reduced abundance of endogenous MCU in Barth syndrome patient cells that are deficient in CL.

We have recently published a paper showing the rescue of mitochondrial function in genetic models of copper deficiency by anti-cancer drug elesclomol. (Soma et. al., 2018 PNAS). The Welch foundation grant supported development of some of the assays that were used in this PNAS paper.

IDO GOLDING, Q-1759, Baylor College of Medicine. GENE REGULATION BY TRANSCRIPTION FACTORS: SINGLE-MOLECULE CHEMISTRY IN THE CELL.

Current research: By combining single-molecule RNA detection with gene-locus labeling, we are now able to measure the transcriptional activity of a single copy of a gene of interest in individual *E. coli* cells, in both live and fixed samples. These measurements allow us to explore multiple questions that cannot be addressed when using whole-cell measurements, including: (1) How does gene activity change during the cell cycle? Is transcription coupled to specific events such as gene replication? (2) What is the relation between the activities of multiple copies of the same gene, which are naturally present in the same cell as part of the bacterial cell cycle? Do the copies act independently or are they correlated? (3) What is the life history of RNA in the cell? What fraction of its lifetime is spent attached to the template gene, versus diffusing in the cytoplasm? Can nascent (actively transcribed) and mature RNA be found anywhere in the cell, or do they exhibit spatial preferences?

Publications: During this grant year, we published two papers describing work funded in part by Welch:

- (1) Sivaramakrishnan et al. (*Nature* 2017) is part of our continuing collaboration with the group of Christophe Herman (BCM), who are studying the coupling between transcription fidelity and genome maintenance in *E. coli*. In this latest paper, we contributed the stochastic modeling of DNA repair at the single-cell

level. The model was used to interpret and parametrize experimental deep-sequencing data describing chromosome degradation following a double-strand DNA break. (2) *Golding (Current Opinion in Microbiology 2018)* briefly reviews the recent shift in our understanding of cellular heterogeneity, a shift which allows us to reevaluate the precision at which gene regulation takes place at the single-cell level.

ELIZABETH J. GOLDSMITH, I-1128, The University of Texas Southwestern Medical Center. KINETIC AND CHEMISTRY OF THE p38 MAPK CASCADE.

This past year, we have continued our work on interactions between the MAP2K MEK1, and its activation by MEKK1 and B-Raf. One publication on this study is now in print. We are continuing to work on characterizing cancer mutants that shed light on the interactions of the wild-type protein in the MAP kinase cascade. A recent publication from Neal Rosen's group at Sloan Kettering has enumerated additional cancer mutants, including MEK1/Y130C, MEK1/P124L, MEK1/K57N as well as deletion mutants. We have had clones synthesized for these mutants and are characterizing them. As with the earlier analyzed MEK1/F53L, we have found that these mutants are destabilized with respect to thermal denaturation.

In addition, we have started on the new grant funded from 2018-2021, which concerns how the MAP3K ASK1 is activated by osmotic pressure. We have obtained clones for the full length protein and for the regulatory and kinase domains expressed separately. Structures are available, and our hypothesis is that the regulatory domain changes shape on exposure to crowding agents. We are carrying out crystallization trials and stabilization assays on the regulatory domain and the kinase domain. As hypothesized, PEG400 stabilizes the regulatory domain with about 4 deg C. PEG400 sharpens the denaturation curve for the phosphorylated form, and destabilizes by about 1 deg C the unphosphorylated form. These initial results are encouraging that our model is correct.

JOHN B. GOODENOUGH, F-1066, The University of Texas at Austin. INFLUENCE OF COUNTER CATION IN MIXED-METAL OXIDES.

Localized 4d electrons of Rh4+ have spin-orbit coupling of strength intermediate between that of Co4+ and Ir4+, but the electronic properties of isostructural oxides of Rh4+ have not been studied because rhodium is expensive and isostructural SrRuO3 perovskites can only be prepared under very high pressure. We have prepared not only the high-pressure SrRhO3 perovskite phase, but also the post-perovskite phase and begun measurement of several of their physical properties. In another study, we have shown that CaMnTi2O6, which contains columns of Mn2+ in face-sharing octahedral sites, undergoes Mn2+ displacements along the columnar axis to create locally electric dipoles. We demonstrated that the Mn2+ displacements become cooperative below a critical temperature TC to give an order-disorder ferroelectric transition rather than the classic cooperative displacive transition below TC as in BaTiO3.

Rechargeable electrochemical cells may be supercapacitors, fuel cells, or battery cells. The different properties of hydrogen-bonded supercapacitors of similar chemistry were shown to be the result of different orientations of the c-axis with respect to the short-dimension of platelet particles. We have developed low-cost bifunctional catalysts for the oxygen-reduction and oxygen-evolution reactions during, respectively, discharge and charge of a rechargeable air cathode and distinguished the catalytic pathways at room-temperature in alkaline solution in battery cells versus PEM fuel cells at 700°C in a rechargeable solid-oxide fuel cell that stores electric power in a chemical bed. We have developed composite polymer-oxide solid electrolytes that are mechanically robust and flexible for all-solid-state rechargeable batteries and shown that alkali-metal anodes can be plated/stripped at low impedance if the alkali-metal wets the solid electrolytes. We have demonstrated sodium and potassium all-solid-state coin cells with composite electrolytes.

PAOLO GRIGOLINI, B-1577, University of North Texas. EMERGENCE OF BIOLOGICAL COMPLEXITY.

The main result has been the formulation of a theory of spontaneous self-organization called Self-Organized Temporal Criticality (SOTC) that applied to neurophysiology sheds light on making decisions under effort, and applied to condensed matter may extend the non-equilibrium processes so as to go beyond the limits of Boltzmann and Arrhenius theories. The new theoretical perspective rests on the role of crucial events [1] which are proven to be the source of multi-fractal processes. SOTC is a new approach to criticality [2] replacing the critical slowing down of the conventional theories with temporal complexity, namely, with randomness hosting crucial events. SOTC is proved to have interesting sociological applications [3] while showing that the adoption of meditation produces neurophysiological effects of the same kind as those generated by addressing a difficult task. This observation leads to the conclusion that these phenomena are much beyond the conventional Hamiltonian approach and suggests that SOTC may replace the traditional Hamiltonian non-equilibrium theories and that this extension should be applied when life processes are involved in the experimental observation [4]. Preliminary results show that SOTC may help to create a bridge between physics and biology leading to establish the crucial role of cooperation for the most elementary biological processes. To support this ambitious conjecture, it is necessary to adopt for the detection of the statistical properties of crucial events the novel technique illustrated in [5]. In fact, neurophysiological and biophysical experiments that must be done to confirm SOTC are expected to be the source of crucial events. Crucial events, which are the source of ergodicity breaking, thereby rendering obsolete the adoption of traditional statistical theories, are the key ingredient for information transport and the success of the research work rests on a very accurate evaluation of their statistical properties.

NICK V. GRISHIN, I-1505, The University of Texas Southwestern Medical Center. DISCOVERING NEW CHEMISTRIES WITH WHOLE GENOME SEQUENCING.

We obtained and published 3 de novo complete genomes, those of *Achalarus lyciades* and of two *Calephelis* species. *Achalarus* is a relative of *Lerema accius*, a species with gene expansion of unusual chitinase-like enzymes that are likely to participate in digestion of cellulose-rich grasses that are used as food plants by their caterpillars. Interestingly, genomic comparison revealed the absence of these proteins in *Achalarus*. *Achalarus* caterpillars feed on nutrient-rich leaves of beans and may not need these enzymes. Analysis of genomes of *Calephelis* revealed a number of interesting adaptations. We found gene expansions in actin-disassembling factor, cofilin, and chitinase. They may aid molting of caterpillars covered in extensive setae. Furthermore, we continued

development of computational methods for the analysis of these enzymes and applied these methods to classify cell surface and secreted proteins in *Drosophila*, to assemble proteins into families in our ECOD database, and to analyze evolution of Rossmann-fold-containing proteins in viruses. We also analyzed predictions of effects of mutations in SUMO-conjugating enzyme UBE2I on its function. Finally, we obtained genomic reads of several *Udranomia* species that are very closely related to each other to learn about proteins that differ the most between them and are likely correlated with speciation events. This last study has been published in PNAS.

ARNOLD M. GULOY, E-1297, University of Houston. **CHEMICAL BONDING AND PROPERTIES OF POLAR INTERMETALLICS ALONG THE BORDER BETWEEN METALS AND NONMETALS.**

The highlight of this year's accomplishments is the discovery of a new metastable germanium allotrope, Ge (α P32), synthesized as polycrystalline powders and single crystals from the mild-oxidation and delithiation of a Zintl phase, $\text{Li}_7\text{Ge}_{12}$, in ionic liquids. Its crystal structure, from single crystal x-ray diffraction, features a complex low symmetry covalent network of 4-bonded Ge derived from the topotactic condensation of $[\text{Ge}_{12}]_7$ - layers in $\text{Li}_7\text{Ge}_{12}$. It is a narrow direct gap semiconductor ($E_g = 0.33$ eV) and transforms exothermically and irreversibly to α -Ge at 363° . This demonstrates the potential of ionic liquids as reactive media in the mild oxidation of Zintl phases to new highly crystalline modifications of elements and simple compounds. A report on this allotrope was published as a communication in JACS.

Another highlight this year is the discovery and synthesis of a novel intermetallic lanthanum silver germanium oxide, $\text{La}_{26}\text{Ag}_6\text{Ge}_{20}\text{O}_5$. It features an intergrowth structure of novel La_{18}O_5 , lanthanum suboxide clusters embedded in a network of Ag-Ge. La_{18}O_5 represents a unique example of an interstitially-stabilized reduced lanthanum condensed cluster derived from the condensation of 5 La_6O octahedral clusters in a tetrahedral manner. It also undergoes superconducting transition at ~ 5 K. Further studies on complex polar (salt-like) intermetallic carbometallates, containing lithium, alkaline earth metals, transition metal (Ni) and carbon resulted in the synthesis of novel TM carbides (carbometallates) with unique TM-carbon anions: a linear $[\text{Ni}(\text{C}_2)_2]_6$ -anion in $\text{Li}_2\text{Ca}_2\text{NiC}_4$; and a triangular planar $[\text{Ni}(\text{C}_2)_3]_8$ - in $\text{Li}_2\text{Sr}_3\text{NiC}_6$. Manuscripts reporting these new compounds will be submitted soon. A Welch summer scholar (high school), and a German exchange student (diplome) from Univ. of Mainz, worked on these projects and were mentored in 2017-2018.

JASON H. HAFNER, C-1761, Rice University. **SURFACE ENHANCED SPECTROSCOPY FOR BIOMEMBRANE STRUCTURE.**

The structural analysis method was improved to consider multiple molecules, multiple configurations, and overlapping peaks. The thermophoretic effect of laser-induced heating on the local gold nanorod concentration was studied since it directly impacts the light scattering signal. These improvements were tested on an initial study of the cetyltrimethylammonium bromide (CTAB) layer on gold nanorods, where a structural transition at a CTAB solution concentration of 2 mM was observed as an increase in the tilt angle of the surfactant layer. For the probe di-4-ANEPPS in lipid membranes, five spectral peaks were confidently matched to vibrations calculated with time-dependent density functional theory (TDDFT).

Structural analysis based on these modes revealed that the probe sits with its long axis 54 degrees from the membrane normal. Attempts to solve the z-position of the membrane probe within the lipid membrane by comparing di-4-ANEPPS modes with the lipid headgroup were inconclusive partly due to spectral overlap. Moving forward, deuterated lipids will be employed to spectrally separate the lipid and di-4-ANEPPS peaks. The peptide ovispirin-1 was chosen as a model α helix since it contains a single aromatic residue (tyrosine) that may be observed, and since the structure has been widely studied by methods including vibrational spectroscopy. It was inserted into lipid membranes and new spectral peaks were found in the surface enhanced spectra. They are currently being analyzed and compared to TDDFT calculations to find which can be assigned to amide bands and which possibly assigned to tyrosine.

NAOMI J. HALAS, C-1220, Rice University. **CHEMICAL AND PHOTOPHYSICAL PROPERTIES OF ELECTRON-DELOCALIZED NANOPARTICLES.**

Expanding on the antenna reactor design paradigm, we have developed a simple polyol synthesis as a flexible route to produce Aluminum nanocrystals decorated with eight varieties of size-tunable transition-metal nanoparticle islands, many of which have precedence as heterogeneous catalysts. This makes transition-metal decorated aluminum nanocrystals a promising material platform to develop plasmonic photocatalysis, surface-enhanced spectroscopies, and quantum plasmonics. We developed Terahertz rotational spectroscopy as a new tool for identifying and quantifying the composition of gas phase reactants and products during chemical reactions. This technique provides unambiguous molecular recognition specificity down to less than a nanomole of gas or less than $10 \mu\text{Torr}$ partial pressure.

We have synthesized Aluminum nanorods with polarization dependent plasmon resonances spanning the IR, visible and UV regions. Structural analysis confirms that these rods are single crystalline and have a hexagonal cross section. We continued the investigation of multilayer gold nanoparticles and their plasmonic properties relevant to fluorescence enhancement and local photothermal/magnetic interactions with nearby molecules.

Polycyclic aromatic hydrocarbon (PAH) molecules, typically consist of 50 or fewer atoms. With the addition or removal of a single electron, these molecules support molecular plasmon resonances in the visible region of the spectrum. We probe the plasmon dynamics in these quantum systems by measuring the excited state lifetime of three negatively charged PAH molecules. These systems exhibit rapid decay dynamics due to the de-excitation of multiple electron-hole pairs through molecular plasmon dephasing and vibrational relaxation. This study provides a first look into the distinction between collective and single-electron excitation dynamics in the purely quantum limit and introduces a conceptual framework with which to visualize molecular plasmon decay.

P. SHIV HALASYAMANI, E-1457, University of Houston. SYNTHESIS, CRYSTAL GROWTH, CHARACTERIZATION, AND STRUCTURE-PROPERTY RELATIONSHIPS IN NEW DEEP ULTRAVIOLET NON-LINEAR OPTICAL MATERIALS.

We have synthesized, grown crystals, characterized, developed structure-property relationships, and investigated theoretically several new oxide materials that exhibit second-harmonic generation (SHG). One of our aims is to synthesize new SHG materials that have nonlinear optical (NLO) capabilities in the UV (200-400nm) and deep-UV (< 200nm) regimes. Notable discoveries this year include the synthesis of K₃Sr₃Li₂Al₄B₆O₂₀F, Rb₃Ba₃Li₂Al₄B₆O₂₀F and Pb₂BO₃I. All three materials have very short absorption edges, < 200nm, and exhibit strong powder SHG responses at 1064nm and 532nm. With the two former compounds, we were able to grow large centimeter size crystals and determine its birefringence and SHG limit. K₃Sr₃Li₂Al₄B₆O₂₀F, and Rb₃Ba₃Li₂Al₄B₆O₂₀F are viable materials for frequency doubling 532nm radiation. We also published a Viewpoint in Inorganic Chemistry that describes the characterization requirements for deep-UV NLO materials. We have also published four (4) papers in collaboration. We have expanded our crystal growth capabilities with three high temperature vertical furnaces that will enable us to pull crystals using Czochralski methods. We are continuing our synthetic efforts on the discovery of new materials, their full characterization, and the development of structure-property relationships.

MICHAEL B. HALL, A-0648, Texas A&M University. COMPUTATIONAL CHEMISTRY OF TRANSITION METAL SYSTEMS.

The hydrogen evolution reaction, as catalyzed by two electrocatalysts [M(N₂S₂)-Fe(NO)₂]⁺, [Fe-Fe]⁺ (M = Fe(NO)) and [Ni-Fe]⁺ (M = Ni) was investigated by computational chemistry. As nominal models of hydrogenase active sites, these bimetallics feature two kinds of actor ligands: Hemilabile, MN₂S₂ ligands and redox-active, nitrosyl ligands, whose interplay guides the H₂ production mechanism.

Introducing two electrons and two protons to [Ni-Fe]⁺ produces H₂ from coupling a hydride temporarily stored on Fe(NO)₂ (Lewis acid) and a proton accommodated on the exposed sulfur of the MN₂S₂ thiolate (Lewis base). With more nitrosyls as in [Fe-Fe]⁺, accumulated electronic space in the nitrosyls' p*-orbitals makes reductions easier, but redirects the protonation and reduction to sites that postpone the actuation of the hemilability. Additionally, two electrons donated from two nitrosyl-buffered irons, along with two external electrons, reduce two protons into two hydrides, from which reductive elimination generates H₂.

Carbon-hydrogen bond activation of alkanes by Tp*Rh(CNR) (Tp' = Tp = trispyrazolylborate or Tp* = tris(3,5-dimethylpyrazolyl)borate) were followed by time-resolved infrared spectroscopy (TRIR) in the (CNR) and (B-H) spectral regions on Tp*Rh(CNCH₂CMe₃), and their reaction mechanisms were modeled by density functional theory (DFT) on TpRh(CNMe). The major intermediate species were: 3-1-alkane complex (1); 2-2-alkane complex (2); and 3-alkyl hydride (3). Calculations predict that the barrier between 1 and 2 arises from a triplet-singlet crossing and intermediate 2 proceeds over the rate-determining C-H activation barrier to give the final product 3. The activation lifetimes measured for the Tp*Rh(CNR) and Tp*Rh(CO) fragments with n-heptane and four cycloalkanes (C₅H₁₀, C₆H₁₂, C₇H₁₄, and C₈H₁₆) increase with alkanes size and show a dramatic increase between C₆H₁₂ and C₇H₁₄.

JOHN C. HARDY, A-1397, Texas A&M University. NUCLEAR DECAY STUDIES.

We continue our measurements and analysis of superallowed beta-decay transitions, which are aimed at testing the universality of the weak interaction. We have published a precise measurement of the half-life of ³⁰S and are completing analysis of a new measurement of the branching ratio for ¹⁰C beta decay. The analysis of ²⁶Si decay, which is the Ph.D. thesis project of M. Bencomo, is complete and being written up. A manuscript describing our results for the decay of ³⁴Ar only awaits a further measurement (now scheduled at Notre Dame University's accelerator facility) aimed at clarifying an ambiguous feature brought to light by our analysis. Work also continues on the decay of ⁴²Ti: We have measured its half-life and are poised to complete a measurement of its branching ratio. These last three decays, of ²⁶Si, ³⁴Ar and ⁴²Ti, together with that of ³⁸Ca, which we have already published, are mirrors to already well-studied superallowed decays; once the superallowed transitions in these four mirror pairs have been fully characterized – our goal for next year – we will be able to apply important constraints to the calculated isospin-symmetry-breaking corrections that contribute to the universality test. In the second component of our program, we have completed a measurement of the internal-conversion-coefficient (ICC) for the E3 transition in ¹⁰³Rh and are well advanced on the measurement of an M4 transition in ⁹³Nb. When completed, we will have made precise ICC measurements of high multipolarity transitions in 10 nuclei spanning 41 = Z = 78. This will constitute the most precise and comprehensive test of ICC calculations ever made. Our early results prompted the National Nuclear Data Center to change the calculations used by its evaluators in producing nuclear decay schemes for widespread general use. When completed, our results covering a wide range of nuclei will potentially lead to further refinements in the calculations.

RASKIA M. HARSHEY, F-1811, The University of Texas at Austin. A RADICAL PROPOSAL FOR HOW TRANSMEMBRANE TRANSIT OF H⁺-IONS CAN GENERATE AN OSCILLATING ELECTRIC FIELD FOR DRIVING ROTATION OF THE FLAGELLAR MOTOR.

CheY~P modulates motor behavior to control chemotaxis. We have made two discoveries. (1) When bacteria move in a dense group known as a 'swarm', their chemosensory physiology is altered. The flagellar motors run at faster speeds in these bacteria and the levels of the CheZ phosphatase are elevated, reducing the levels of CheY~P and resulting in a reduced tumble bias and a reduced chemotactic performance. This behavior persists for long periods, showing that the chemotaxis signaling pathway is reprogrammed for swarming. We suggest that swimmers repurpose their chemosensory pathway to optimize collective motion for varied outcomes such as colony expansion, search for nutrients and/or their known high tolerance to antimicrobials. (2) We have discovered that the chemosensory pathway is important for the high tolerance to antibiotics exhibited by the swarm. Using fluorescence microscopy, we took a first look inside a 3D swarm, and found a novel architecture to the colony. We found that secreted bio-surfactants keep bacteria away from the swarm-air upper boundary, and added antibiotics keep them away from the swarm-surface lower boundary. Maximal cell occupancy is at an intermediate region between the upper and lower swarm boundaries. This arrangement may offer maximal protection from environmental assaults at both boundaries. Formation of the

antibiotic-avoidance zone is dependent on a functional chemotaxis signaling system, in the absence of which, the swarm loses its high tolerance to the antibiotics. A bacterial chemotactic response to antibiotics has not been observed in liquid, suggesting that this response is an emergent property of the swarm.

J. D. Partridge, N. Q. Nguyen, Y.S. Dufour and R. M. Harshey. *Escherichia coli* repurposes chemotaxis for swarming. Under revision for *Mbio*.

J. D. Partridge, G. Ariel, O. Schwartz, A. Be'er, and R. M. Harshey. Bacterial swarming in three dimensions: Implications for antibiotic tolerance. Under review for *Sci. Reports*.

P. JOHN HART, AQ-1399, The University of Texas Health Science Center at San Antonio. IN SILICO SCREENING FOR INHIBITORS OF CARDS TOXIN FROM *M. PNEUMONIAE*.

Differential Scanning Calorimetry (DSC) and Thermal Shift Assay (TSA) was used to assess compound binding to CARDS toxin (CARDSTx). We found ribavirin and compound 784870 induced shifts of CARDSTx thermal stability indicating binding. Predicted binding modes and potency of compounds raised a question of model accuracy. The CARDSTx structure suggested the D1/D2 binding site contains water molecules that might play a crucial role in determining which compounds can bind strongly.

Therefore, we investigated stability of water molecules in the pocket. We conducted molecular dynamics (MD) simulations of unbound CARDSTx to identify non-uniform distribution of water residence times and positions of polar atoms that a putative ligand should have to achieve stronger binding. Analysis of the MD trajectories derived concerted motions in the protein. These data will be used to improve the binding hypothesis to the D1/D2 pocket and increase scoring accuracy to be derived from further virtual screening. Success of the virtual screening critically depends on chemical space for ligand selection. To derive a wider chemical space with improved physico-chemical properties and more diverse chemotypes, we preprocessed a database of over 175,000,000 chemical structures. The database was enumerated using a combinatorial approach, filtered by synthesis feasibility, subjected to 2D to 3D conversion, ADME-Tox properties prediction and is now ready for vHTS. We will use the improved binding model screen and select 20-50 candidates for evaluation by TSA. In addition to the in silico experiments, we found a suitable in vitro strategy (DNA-encoded Chemistry Technology, DEC-Tec) to rapidly screen a library of one billion drug-like compounds to identify binders to CARDSTx. DEC-Tec has advantages of cost-effectiveness and screening in solution. DEC-Tec technology will be applied to CARDSTx for compound screening followed by crystallization and structure determination of complexes with hit compounds.

JEFFREY D. HARTGERINK, C-1557, Rice University. SYNTHESIS OF NANOSTRUCTURED ORGANIC MATERIALS VIA SELF-ASSEMBLY.

Our published work this year focused on our MultiDomain Peptides (MDPs) which are short synthetic peptides that are designed to self-assemble into nanofibers and then thixotropic hydrogels. These three publications demonstrate the important applications that our MDPs are now able to be applied toward after many years of fundamental research supported by the Welch Foundation. Our publication "Nanofibrous peptide hydrogel elicits angiogenesis and neurogenesis without drugs, proteins, or cells" (*Biomaterials*) brings our self-assembling system to in vivo testing. We found that our nanofibrous system is rapidly infiltrated with host cells which then begin a cascade of cytokine and growth factor production which recruit vascularization and neurogenesis. Amazingly, this biological reaction takes place in response to the self-assembled hydrogel alone without the need for drugs or exogenous cells. "Multidomain Peptide Hydrogel Accelerates Healing of Full-Thickness Wounds in Diabetic Mice" (*ACS Biomater. Sci. Eng.*) takes this approach one step further and demonstrates that in a model of diabetic ulcers that our nanostructured materials are able to accelerate healing by many different metrics including wound closure, vascularization, nerve regeneration and hair follicle formation. Finally in "STINGel: Controlled release of a cyclic dinucleotide for enhanced cancer immunotherapy" (*Biomaterials*) we apply the self-assembling MDPs to immunotherapy drug delivery. We combine MDPs with a new immunotherapy agent, a cyclic dinucleotide (CDN) to make a new material we call "STINGel", to treat a difficult model of oral cancer. We found that 60% of mice treated with STINGel recovered compared to only 10% treated with CDN alone. These mice were found to be immune to further dosing with the cancer, a hallmark of successful immunotherapy.

KADEN HAZZARD, C-1872, Rice University. ULTRACOLD NONREACTIVE MOLECULES: FROM COLLISION COMPLEXES TO COMPLEX MATERIALS.

After year 3, research is ahead of schedule. In the first two years, we derived an effective model for many NRMs in an optical lattice, incorporating a variety of models of the chemical processes, with at most two molecules per site [PRL 116, 135301 (2016), PRA 95, 043635 (2017), PRA 95, 043636 (2017) mostly cover this]. In year 3, we have worked out many consequences of these models, and completed the remaining objectives for the grant.

Specifically, we have (1) gone beyond the phenomenological collisional models to ones grounded in our microscopic understanding of the molecular interactions, and (2) determined an effective model suitable for three molecules on one lattice site. I will describe one example. A typical phenomenological used takes random matrix theory for two-molecule bound states. We have found that the simplest realistic microscopic model of molecular interactions gives spectral statistics that are random matrix like, but with significant corrections. This is the first evaluation of the validity of the oft-used random matrix description for the chemical properties. These results are being written up for publication.

Our results have unexpectedly also opened new, exciting avenues of research in measuring and controlling chemical systems, and in many-body physics. As one example, in chemistry, using our finding that chemical dissociation reactions can be probed with spectroscopic techniques at an unprecedented energy resolution -- 10 or more orders of magnitude more accurately than previously possible -- we are now developing protocols to use this to produce ultracold polyatomic molecules.

This new area is being actively studied by our group. Investigating the new potential to understand and control chemistry using the exquisite capabilities of ultracold matter using the ideas developed in this project will be a major component of the follow-up Welch award (2018-21).

ADAM HELLER, F-1131, The University of Texas at Austin. ELECTROCHEMICAL AND BIOELECTROCHEMICAL APPLICATIONS OF METAL OXIDE TEMPLATED CARBON ELECTRODES.

1. The prevalence of type 2 diabetes (T2D) is increasing, afflicting > 7 % of the world's people. In T2D inefficient cellular insulin-utilization increases the insulin demand; the demand is unmet when insulin-secreting pancreatic beta-cells die. The most widely used submicron-sized crystalline material is "white" TiO₂, its 200-300 nm particles tailored to optimally scatter visible light. It is used in drinks, foods, toothpastes, cosmetics, medications, indoor wall paints, paper and plastics. Its production increased in the past 50 years from 2 to 6 million tons/year. Earlier studies have shown that TiO₂ enters the bloodstream when inhaled or ingested. TiO₂ is phagocytized by leukocytes, and activating the NLRP3 inflammasome it initiates an inflammatory cascade leading to the death of proximal cells. In a pilot study of 11 pancreatic specimens we found over 200 million TiO₂ particles per gram in the pancreas of each of 8 T2D donors, but not in the pancreas of any of 3 nondiabetic donors. Apparently, pancreatic TiO₂ crystals cause or propagate T2D. (Heller, A. et al., Association of Type 2 Diabetes with Submicron TiO₂ Crystals in the Pancreas. *Chem. Res. Toxicol.* 2018, Ahead of Print.)

2. FreeStyle Libre of Abbott Diabetes Care is based on earlier Welch Foundation sponsored studies of polymeric hydrogels electrically wiring redox enzymes. It became this year the world's most widely used continuous glucose monitor.

3. Studies of carbon- and other- nanoscale lithium and sodium battery materials continued. (2-(Youn, D.H. et al. Enhanced Electrochemical Performance of a Tin-Antimony Alloy/N-Doped Carbon Nanocomposite as a Sodium-Ion Battery Anode. *ChemElectroChem* 2018, 5 (2), 391-396; Lin, J. et al., Self-Assembled Cu-Sn-S Nanotubes with High (De) Lithiation Performance. *ACS Nano* 2017, 11 (10), 10347-10356. Rodriguez, R. et al., In Situ Optical Imaging of Sodium Electrodeposition: Effects of Fluoroethylene Carbonate. *ACS Energy Lett.* 2017, 2 (9), 2051-2057).

GRAEME HENKELMAN, F-1841, The University of Texas at Austin. DESIGN OF MATERIALS FOR ENERGY CONVERSION AND STORAGE.

Computational Methods: This past year, I co-edited a special edition in JCP with Cecelia Clementi to highlight new computational methods for calculating reaction pathways [Clementi17]. One example takes energetics of Li binding and diffusion in LiFePO₄ and uses kinetic Monte Carlo model to model the charge and discharge kinetics over experimental time scales [Xiao18]. This study provided strong evidence for a kinetically stabilized lithium striped phase at high charging rates.

Catalysis: With the Crooks group, we explored a synthetic method in which electrochemical pulses were used to deposit self-terminated monolayers of Pt on Au. This method worked well on bulk electrodes, but as we show in our JACS paper [Lapp18] the structure of nanoparticles is significantly more complex. With the Mullins group we studied the mechanism of ethanol dehydrogenation on alloy surfaces [Evans17, Li17] and oxygen evolution on CeOx and CoOx electrocatalysts [Kim18]. With the Humphrey group we designed classically immiscible Rh based alloy particles for hydrogenation reactions [Piburn18, Li18]. Perhaps the most notable work this year was with the Bard group, reported in JACS [Kai17], in which experiment and theory point to a surprising mechanism for CO₂ reduction in which the CO₂ molecule accepts an electron before adsorbing on the catalytic surface.

Battery materials: With the Mullins group we studied a copper tin sulfide constructed in a hierarchical tubular structure with good cycle life despite large volume expansion upon lithiation [Lin18]. But the development that I am most excited about is the recruitment of outstanding postdoc, Ieuan Seymour. Ieuan is an expert in both the synthesis and modeling of battery materials. He came to UT with his own project – to make nanocomposites of layered and rocksalt metal oxides, with the idea that the former can provide high a rate capability and the later particle stability. I will report the results next year!

W. MIKE HENNE, I-1873, The University of Texas Southwestern Medical Center. NOVAL PATHWAYS OF ER-ENDOLYSOSOMAL INTER-ORGANELLE COMMUNICATION.

Welch funds my biochemical research on PXA domain-containing proteins. This project was originally allocated to my postdoctoral fellow Dr. Lydia (Yang) Liu, and later to my post-doc Dr. Hanaa Hariri. Both have completed their Aims as outlined, and published first author papers on their findings (Bryant & Liu, *Human Molecular Genetics*, 2018; Hariri, *EMBO Reports*, 2017). In addition, we have prepared two follow-up manuscripts that we are preparing to submit in the coming weeks that continue our dissection of PXA domain proteins in lipid metabolism and inter-organelle crosstalk (Datta, in preparation; Hariri, in preparation).

Our group characterized yeast PXA proteins Mdm1 and Nvj3 as residents of the ER-vacuole/lysosome membrane contact site (MCS), and demonstrated that Mdm1 functions as a tether connecting the ER and vacuole (Henne, *JCB*, 2015). To determine whether the Mdm1 PXA domain binds to lipids (Aim 1), we expressed and purified PXA domain and developed in vitro lipid binding assays. These assays reveal the PXA domain binds to lipids with preference for mono-acyl fatty acids, diacyl neutral lipids like DAG, and sterols. We have discovered that the PXA proteins associate with lipid droplets (LDs) in living cells and control LD biogenesis during stress (Hariri, *EMBO Reports*, 2017). Our current manuscript features a mechanistic dissection of the PXA-lipid interaction, and how Mdm1 interacts with fatty acyl-CoA ligases to promote fatty acids into lipid droplets (LDs) to maintain ER homeostasis (relevant to Aims 2 & 3) (Hariri, et al, in preparation).

We have also partnered with a clinical collaborator in UCL, London and published a study examining human Mdm1 homolog Snx14 in pediatric cerebellar ataxia SCAR20. We find that Snx14 functions in ER-LD inter-organelle crosstalk and LD formation (Bryant & Liu, *HMG*, 2018). We are preparing a manuscript using APEX technology to further dissect the mechanisms of Snx14 function in LD biogenesis (Datta, in preparation).

RYAN E. HIBBS, I-1812, The University of Texas Southwestern Medical Center. STRUCTURAL PRINCIPLES OF INHIBITORY NEUROTRANSMITTER RECEPTOR MODULATION.

We have made rapid progress in structural biology of the principal GABA-A receptor subtype in this second year of funding. This receptor comprises alpha1, beta2 and gamma2 subunits in a pentameric arrangement. We used Fab antibody fragments described at the end of the last progress report to form a complex with our recombinant GABA-A receptor for the purposes of electron microscopy analysis. We optimized sample preparation for single particle cryo-EM studies and over the course of a few months collected a large dataset on the receptor sample. We processed this dataset and obtained a receptor reconstruction to an overall resolution of 3.9 Angstrom, with local resolution near the small molecule binding sites at 3.0A or better. This resolution allowed us to build and refine the first atomic model of a physiological assembly of a GABA-A receptor. We have just had a manuscript on this work accepted for publication as an Article in Nature. In this paper we describe principles of ligand recognition for GABA, the endogenous neurotransmitter, and benzodiazepines, one of the most popular prescription drug classes. We are now building off this first structure with (1) structures of the receptor in a lipidic environment (the first structure was in detergent) and (2) structures of additional ligand complexes.

LEA HILDEBRANDT RUIZ, F-1925, The University of Texas at Austin. EFFECTS OF CHLORINE ATOMS ON TROPOSPHERIC OXIDATION CHEMISTRY.

We have conducted laboratory chamber experiments on the oxidation of isoprene, toluene, alpha-pinene and different alkane precursors, all initiated by chlorine atoms (Cl). One manuscript (focused on isoprene + Cl) was published and two manuscript (focusing on toluene + Cl and on alkanes + Cl) were submitted for publication. A second manuscript on alkanes + Cl and a manuscript on alpha-pinene + Cl are expected to be submitted in this second grant year.

Results from the isoprene + Cl experiments included observation of multi-generational chemistry, including ions consistent with hydroperoxides, chloroalkyl hydroperoxides, isoprene-derived epoxydiol (IEPOX), and hypochlorous acid (HOCl). This is evidence of secondary OH production and resulting chemistry from Cl-initiated reactions. Results from alkane + Cl experiments included observed secondary organic aerosol mass yields (0.16 to 1.65) higher than those for OH-initiated oxidation of alkanes (0.04 to 0.35). Chlorinated organics were observed, which likely originated from chlorine addition to the double bond present on heterogeneously produced dihydrofurans. A two-dimensional thermogram representation was developed to visualize composition and relative volatility of organic aerosol components using unit-mass resolution data from a chemical ionization mass spectrometer. Aerosol mass yield and oligomer formation were suppressed under humid conditions relative to dry conditions. Results from the toluene + Cl experiments included that the presence of nitric oxides (NOx) appears to slow down the chemistry, presumably due to the formation of ClNO2 which serves as temporary sink of Cl and NOx. Mass spectrometer data suggested that secondary organic aerosol (SOA) formed had high oxidation state, and that the bulk organic composition was different for SOA from Cl-dominated reactions than for SOA from OH-dominated reactions.

CHRISTIAN B. HILTY, A-1658, Texas A&M University. CHARACTERIZATION OF OLEFIN METATHESIS USING DISSOLUTION DYNAMIC NUCLEAR POLARIZATION.

For the ring-opening metathesis polymerization reaction catalyzed by second and third generation (G2 and G3) Grubbs catalysts, experiments using various catalysts concentration are performed. Reactions were observed by real-time NMR with ¹³C hyperpolarization of the monomer norbornene. A saturation-like behavior was found in the dependence of the reaction rate on catalyst concentration for G3. This behavior is explained by the inhibition of the reaction through re-binding of a pyridine ligand that is lost during catalyst activation. This NMR based titration is facilitated by hyperpolarization, which enables to measure the reaction at low monomer concentration to avoid the formation of polymer gel during an on-going reaction. We are proposing a new kinetic model that describes the observed NMR signals and includes a binding equilibrium for this ligand. The propagation rate constant determined with this model was then used to calculate the initiation rate constant in the G2-catalyzed reaction, under the assumption that the active species of G2 and G3 catalysts are identical. A related Hoveyda-Grubbs catalyst was used for to our knowledge the first studies of catalyst directly hyperpolarized with dissolution dynamic nuclear polarization (D-DNP). Hyperpolarized signals were observed for various ¹³C atoms of the ligands. In the presence of amine compounds that deactivate the catalyst, broadening of these signals was observed. Line shape analysis is applied for the determination of the corresponding exchange rates from hyperpolarized NMR spectra. Further experiments on co-polymerization of norbornene with cyclooctene using G3 catalyst, first reported in the previous period, were performed to determine self-propagation and cross-propagation rate constants from the time-evolution of NMR signals. The results show preferential self-propagation for norbornene, and preferential cross-propagation for cyclooctene concomitant with a higher reactivity ratio for norbornene.

DAVID M. HOFFMAN, E-1206, University of Houston. SYNTHESIS OF TRANSITION METAL COMPLEXES WITH DI-ANIONIC TRIDENTATE Pincer LIGANDS.

Since 1991, 84 publications acknowledging Welch Foundation support have been published. Over the past 27 years, Welch funds have been used to support dozens of postdoctoral researchers, graduate students, and undergraduate students. In this final year of support, work included setting up new equipment to allow the continuation of research, which will include preparing for publication compounds synthesized with previous grant support (e.g., the dimers [Cr(μ-N=C-t-Bu2)(N=C-t-Bu2)]₂, [Y(μ-N=C-t-Bu2)(N=C-t-Bu2)]₂, and {Y[μ-N=C(t-Bu)(Ph)][N=C(t-Bu)(Ph)]₂}₂, and the square-planar cobalt (II) hydrazonide complex, Co[CH₂C(t-Bu)=NNMe₂]₂).

GARY CHUNG HON, I-1926, The University of Texas Southwestern Medical Center. EPIGENETIC CONTROL OF NON-CODING GENE REGULATION.

Completion of Aim 1. We have designed, tested, and optimized a strategy to systematically clone and functionally test a diverse library of protein effectors of enhancer activity. This strategy has several key capabilities. First, we use a retroviral expression backbone to deliver robust expression of cloned integrated proteins. Second, this Gateway-compatible expression construct enables the high-throughput cloning of arbitrarily-sized protein libraries. Third, the cloned proteins are fused to the bacteriophage coat protein MCP, which mediates recruitment of the proteins to dCas9-bound sgRNAs that are engineered to contain two hairpin MS2 RNA aptamers. Fourth, we have placed a polycistronic blasticidin resistance gene downstream of the MCP fusion, allowing for cell selection and accurate quantification of viral titer. Our tests indicate that 1) the vector is compatible with CRISPR-mediated expression perturbation and 2) we can use a pooled homology based cloning strategy to create MCP-fused TF libraries and over- express them in human cells.

Tagging genes for Aim 2. To implement a fast readout for altered enhancer activity upon protein effector recruitment, we are using GFP to tag genes with known enhancers. We have successfully tagged HBE1, FADS1, FTH1, and STXBP5 in K562 cells. We have isolated multiple independent clones for each and verified endogenous in-frame tagging with Sanger sequencing and functional testing by CRISPRi.

Discovered critical constraints for single-cell barcoding (for Aims 2 and 3). Our first-generation system relied on the detection of distally located genetic barcodes as an indirect proxy of perturbation identity. Since barcodes are often several kilobases from their corresponding perturbations, viral recombination- mediated swapping of barcodes is feasible, causing recombination rates as high as ~50%. Our barcoding strategy (Aim 1) circumvents this problem. This work has been accepted for publication.

LORA V. HOOPER, I-1874, The University of Texas Southwestern Medical Center. ENGINEERING ANTIBACTERIAL LECTINS FOR SPECIFIC TARGETING OF ANTIBIOTIC-RESISTANT BACTERIA.

During the previous two years of this project, we discovered a new family of small membrane-toxic proteins that bind to bacteria and can serve as platforms for further engineering of novel antibacterial proteins. This is the resistin-like protein (RELM) family, members of which are related to resistin, a cytokine that plays a role in glucose homeostasis. During the past year, we have further characterized the bactericidal activity of these proteins, finding that they target a broad range of Gram-negative bacteria that colonize the intestine. We defined the mechanism of bactericidal activity by showing that members of the RELM family form transmembrane pores that permeabilize bacterial membranes. These findings are now published in the Proceedings of the National Academy of Sciences (2017). We are currently working to re-engineer the bacterial binding function of key RELM family members to recognize antibiotic resistant bacteria.

In addition, we have discovered another novel family of intestinal antimicrobial proteins that represent yet another platform for the engineering of novel antibacterial proteins. These proteins are members of the small proline-rich protein (Sprr) family and are expressed at body surfaces such as the skin and the intestine. We are currently characterizing the spectrum of antimicrobial activity for key Sprr proteins and identifying the mechanisms that underlie their antimicrobial activity. We also aim to perform structural studies of these proteins in the near future.

Finally, this award has supported related studies on antimicrobial protein function in the intestine (Bel et al., Science 2017) and how intestinal lipid metabolism is regulated by gut bacteria (Wang et al., Science 2017). We have also participated in a group of collaborative studies with Sebastian Winter's group in the UTSW Department of Microbiology that center on metabolic pathways of gut bacteria. This work has resulted in three co-authored publications.

JULIA W.P. HSU, AT-1843, The University of Texas at Dallas. SULFUR POISONING OF COMPLEX OXIDE CATALYSTS FOR NITRIC OXIDE (NO) OXIDATION: EFFECT OF CRYSTAL STRUCTURE AND STOICHIOMETRY.

Correctly identifying the surface adsorbed species and active sites is critical in elucidating reaction mechanisms and designing a better catalyst. We synthesized mullite-type of RM_2O_5 compounds with $R = \text{Sm, Bi, Y, Gd, Pr}$ and $M = \text{transition metals, Mn and Fe}$, as well as SmMnO_3 perovskite, and various binary oxides by solution methods, to study the roles of M and R elements and the effects of crystalline structure. The oxides were characterized using three groups of techniques: 1) X-ray diffraction and transmission electron microscopy for their crystalline structure, 2) N_2 adsorption isotherms for their surface area and particle size, and 3) Low-energy ion spectroscopy (LEIS) and X-ray photoelectron spectroscopy (XPS) for surface composition and oxidation states of the metal cations. NO adsorption, evolution, and desorption on the catalyst's surface were probed by characteristic vibrational frequencies in Fourier-transform infrared spectroscopy (FTIR), confirmed with XPS measurements and DFT modeling. Nitrates were found to be the stable intermediates. The thermal stability and evolution of surface adsorbed species was probed by in situ heating in FTIR and XPS chambers and thermal programmed desorption experiments. DFT calculations are indispensable in identifying the surface species, the active sites, and the reaction mechanisms. Our results suggest lattice oxygen, rather than transition metal sites, are the active sites for this type of catalysts. This finding is a paradigm shift in heterogeneous oxidation reactions. Our results over the three years of the Welch grant has generated four published papers (and two more in progress), an invited talk, a contributed talk, and two posters. Three PhD students, a postdoc, and three high school students participated in this project. Sampreetha Thampy, who was supported mainly by this grant, will defend her PhD dissertation in March 2018.

RANDALL G. HULET, C-1133, Rice University. UNIVERSAL TRIATOMIC MOLECULES BY ASSOCIATION OF ULTRACOLD ATOMS.

We have completed a major experimental project this year on the effects of modulated interactions in Bose-Einstein condensates (BEC). The BEC consists of ultra-cold atoms cooled to quantum degeneracy. In this work, we showed how collective surface waves known as Faraday waves are excited by the modulation of the interactions between atoms. When driven at frequencies that are near resonant with normal modes, sound waves are generated and interfere

to produce a regular pattern in the density of the BEC. In our case, the BEC is confined to a highly elongated trap, and the resulting Faraday pattern appears as a standing wave along the axial direction of the BEC. Faraday waves were first discovered by Michael Faraday in 1838, when he observed that spatial patterns developed on the surface of a fluid contained in a bucket, whose vertical position was rapidly modulated. We obtained the spectrum of the Faraday waves, and measured the time scales for their emergence.

In a second part of this project, we modulated at frequencies well below the resonances corresponding to the normal modes of the confined BEC. In this case, no periodic pattern was observed, but when the modulation was sufficiently strong and long, the condensate broke into isolated density islands whose size distribution appeared to be random. Our theoretical collaborators found that this "granulation" is a quantum effect whose description goes beyond the standard mean-field model. This is the first time that quantum granulation has been observed.

Finally, we believe that we have solved a particularly pernicious long-standing noise problem in our BEC apparatus, in which the condensates acquired a random initial momentum and position. We determined that the problem was caused by vibrations and acoustic noise connected to the water cooling in of our high-current magnetic coils. We have put the most sensitive part of the apparatus on a separate optical platform that is isolated by sorbothane feet.

SIMON M. HUMPHREY, F-1738, The University of Texas at Austin. DESIGN AND SYNTHESIS OF NEW METALLOLIGANDS FOR THE CONSTRUCTION OF PHOSPHINE COORDINATION MATERIALS WITH ADVANCED SOLID-STATE PROPERTIES.

In the past grant year, we have significantly advanced several parallel areas of interest and also launched a new direction; since 7/17, we have published nine new articles, while five others are in review or under revision.

Following earlier successes using phosphine ligands to prepare novel metal-organic framework (MOF) materials, we developed routes to previously reported phosphines with extended biphenyl and hetrocyclic substituents, which are designed to result in MOFs with larger pores. This has proven an effective strategy: we showed the first example of a MOF with a built-in trans-bis(phosphine) coordination pocket, which could be post-synthetically functionalized in the solid-state with Au(I) or Cu(I). The resulting 'complexes' are in non-equilibrium geometrical states as imposed by the MOF's rigidity. This result (*Angew. Chem.*, 2018) has opened-up new possibilities in terms of using such constructs to generate catalytic materials under strain, which may enable unusual reactivity. Inspired by this result, we then published the first example of an arsine MOF, prepared with a new AsR3 ligand. The MOF has cis- bis(arsine) pockets that were functionalized with Au(I) dimers, resulting in a very short Au-Au distances imposed by the MOF (*JACS*, 2018). We also continue to work with other porous phosphine materials, which show unique solid-state properties (e.g., *Chem. Commun*, 2018; *Polyhedron*, 2018).

In parallel studies, we continue to use the phosphines and other co-polymers as capping agents to prepare nanoparticles with unusual alloy compositions. With Welch support, we have demonstrated the first example of an AgIr alloy (*ACS Catal*, 2018; revision submitted) and also further studied AuRh alloys first reported in 2015, on a single-particle basis, to better understand function at the atomic level. This area of work is currently continuing with an initial assessment of how to prepare Re-based alloy nanoparticles under microwave heating.

GYEONG S. HWANG, F-1535, The University of Texas at Austin. FIRST-PRINCIPLES INVESTIGATION OF THE STRUCTURE, CHEMISTRY AND FUNCTION OF GRAPHENE-LIKE MATERIALS.

Nanostructured carbon materials have been actively explored as a potential candidate to replace platinum-based oxygen reduction reaction (ORR) catalysts in fuel cells. sp²-bonded carbon nanostructures are inherently constituted by largely extended p-conjugation systems, making them essentially unreactive toward molecular oxygen (O₂) in their pristine forms. However, the conjugated p- systems can be severely disrupted with quasi-localized states through dopant incorporation, defect creation, and/or local lattice distortions. The doped, defective and distorted carbon structures are currently thought to be responsible for O₂ adsorption/activation and thus ORR, but the active sites and the exact mechanisms are still uncertain. Using extensive first-principles calculations, we have identified a novel method for the activation of graphene-like structures. This modification creates quasi-localized electron states in the p-conjugated system which are vulnerable to oxidation via O₂. The result is favorable O₂ adsorption, which despite being necessary for ORR activity is not predicted for previously proposed active sites. We have identified the importance of using proper solvation models at the carbon- water interface. Unlike many previous theoretical studies that consistently predict O₂ adsorption to be endothermic on carbon, our study clearly demonstrates that a more accurate description of interactions at the carbon-solvent interface is necessary to properly describe O₂ adsorption. In addition, we have found that more detailed descriptions of charge injection are necessary at carbon-based catalysts, where polarization of the carbon electrode is significant. Our study provides insight into molecular mechanisms underlying the superior ORR activity of nanostructured carbon and also guidelines for the rational design and development of high-efficiency, cost-effective carbon-based ORR catalysts for fuel cell applications.

TATYANA I. IGUMENOVA, A-1784, Texas A&M University. PIN1 "BITES" THE TAIL: REGULATORY ROLE OF THE C-TERMINAL DOMAIN OF PROTEIN KINASE C.

We have made a paradigm-shifting discovery regarding the mechanism of PKC regulation by Pin1: instead of acting as a canonical isomerase, Pin1 acts as a bivalent binding partner of the C-terminal PKC tail (Cterm). In Objective 2, we sought to obtain atomic-level information about Pin1-Cterm interaction.

We pursued two directions: X-ray crystallography and solution NMR spectroscopy. Extensive and exhaustive search for crystallization conditions for the Pin1-Cterm complex produced no hits. We were successful with the solution NMR spectroscopy approach. Using a set of multi-dimensional NMR experiments, we collected all data necessary for the structure determination of the complex. We generated a preliminary NMR structure, which is the first known structure of Pin1 complexed to a bivalent substrate. The structural model revealed two novel features. First, Pin1 adopts a "closed" conformation of the

two domains, which has not been previously observed in solution. Second, the isomerase domain is responsible for the Pin1 interactions with a non-canonical substrate represented by the hydrophobic motif of Protein Kinase C. The hydrophobic motif is a signature motif of AGC kinases. Therefore, this interaction mode could be present in other AGC kinases, thereby significantly broadening the impact of our findings.

We are in the process of finalizing the structure of the complex. This involves (i) obtaining additional inter-molecular restraints, and (ii) refining the orientation of Pin1 domains relative to one another. Additional inter-molecular restraints are being obtained through the use of the C-term regions that are selectively enriched with stable isotopes at specific amino acid positions. The domain orientation is being determined using a set of residual dipolar couplings. Generating the final structure of the complex is a prerequisite for the dynamics studies that are described in Objective 1 of the funded renewal of this proposal.

BRENT L. IVERSON, F-1188, The University of Texas at Austin. A NEW FAMILY OF REPORTING MOLECULES.

Future chemists will routinely create small molecules that self-assemble to form solids with designed and responsive functions. Previously, we discovered a truly remarkable early example of just such a responsive molecular assembly. Our donor-acceptor family of dyad molecules (6-((4-alkoxynaphthalen-1-yl)ethyl)-2-alkyl-1H-benzo[de]isoquinoline-1,3(2H)-dione) create solids including crystals that, without changing macroscopic morphology, can stably and reversibly change from bright orange to yellow when heated or pressed and from yellow back to orange if exposed to solvent vapor! This past year, our work has delivered comprehensive answers to four key issues related to this remarkable behavior: 1. What are the structures of the materials? To date we have solved crystal structures of the orange and yellow forms for 6 and 7 dyad derivatives, respectively, including crystal structures for both the orange and yellow forms for 3 dyad derivatives. 2. Why does the color change? The orange material absorbance is red-shifted due to what spectroscopists call J-aggregate formation and a consequent delocalized excited state, neither of which are present in the yellow solids. 3. Why does this family of dyad molecules have a “split personality”, exhibiting two different stable arrangements in the solid state? The monoimide moiety of the dyad is stable in a face-centered, alternating stacking geometry with the electron-rich naphthyl ether ring of adjacent dyads (yellow material), or in an offset (tilted) monoimide self-stacking mode (orange material). These two geometries are nearly isoenergetic in the solid state. 4. How can the entire assembly undergo such a dramatic change in geometry without disrupting macromolecular morphology? This is truly intriguing, and we have now developed a pioneering model of the molecular motions required for this transition to occur in the solid state. We are preparing an important and extensive manuscript describing these emerging principles.

KHULOUD JAQAMAN, I-1901, The University of Texas Southwestern Medical Center. IN SITU MEASUREMENT OF INTER-RECEPTOR INTERACTION KINETICS ON THE CELL SURFACE.

Our efforts last year were focused on testing the feasibility of our “in situ kinetics framework” when applied to single-molecule data with tracking errors. For this we generated synthetic single-molecule movies from simulated receptor trajectories, and then obtained receptor tracking data from the movies using u-track (Jaqaman et al. Nat. Methods 2008), like experimental movies. These tests turned out to be more challenging than initially anticipated, and consumed most of our efforts last year. However, we have overcome the challenges and can now advance the project as planned, albeit with a delay.

In a nutshell, when we applied our framework to the single-molecule tracking data directly as output by u-track, it failed to retrieve the correct model parameters. We surmised that this failure was due to the difficulty to distinguish between molecular interactions vs. molecules passing by each other in single-molecule data, both of which appear as colocalization events. However, making use of the fact that colocalization events due to molecules passing by each other are shorter-lived than those due to interactions, we devised a scheme to retain – at a statistical level – only those colocalizations due to interactions. Applying our framework to the single-molecule data after the cleanup allowed us to estimate the correct model parameters as accurately as error-free simulated data.

These tests and the associated cleanup scheme had several implications for our studies. First, we are now using similar strategies to clean up our experimental datasets for the receptors VEGFR2 and CD36, as a first step toward applying our framework to experimental data. Second, the tests revealed a minimum signal-to-noise ratio and maximum labeled-molecule density beyond which the tracking errors are too large to clean up, thus guiding our single-molecule experiments.

We are writing a manuscript describing the development and testing of our “in situ kinetics framework.”

MAKKUNI JAYARAM, F-1274, The University of Texas at Austin. MECHANISTIC CHARACTERIZATION AND FUNCTIONAL MANIPULATION OF ACTIVE SITES THAT CATALYZE NUCLEOTIDYL TRANSFER REACTIONS.

A. We are continuing the mechanistic analysis of phage C-31 integrase (a serine site-specific DNA recombinase) using single-molecule tethered particle motion (TPM) analysis. Our initial analyses revealed that compatibility of target DNA sites (attP and attB or attL and attR) for the integrase reaction is controlled at the level of partner site synapsis by the recombination directionality factor RDF. In the physiological context in vivo, RDF promotes phage excision from the bacterial chromosome (attL x attR) and inhibits phage integration (attP x attB). We have continued to address the mechanism of RDF regulation using ‘activated’ variants of the integrase that are able to overcome the requirement of RDF in the attL x attR reaction. We have made significant progress with one such variant Int(E449K). The results so far suggest the mutant protein is able to convert integrase-bound pre-synaptic complexes to functional synaptic complexes at a faster rate. The wild type integrase, by contrast, yields unstable ‘wayward’ synaptic complexes that dissociate without undergoing catalysis. We expect to complete the analysis during the first year of the renewed grant.

B. The Flp site-specific recombinase (a tyrosine site-specific DNA recombinase) plays a key role in amplifying the yeast plasmid 2-micron circle when its copy number drops below the steady state value. Post-translational conjugation of a SUMO moiety at Lys-375 regulates the turnover of Flp in vivo, and prevents runaway increase in copy number. By using a Flp-SUMO hybrid protein, which faithfully mimics the functional characteristics of Flp(K375-

SUMO), we have revealed a second level of regulation at the level of the occupancy of the recombination target sites (FRTs) by the modified protein and its ability to mediate strand cleavage at these sites. The in vitro and in vivo analyses with Flp-SUMO have just been completed, and the manuscript is under preparation.

JENNA JEWELL, I-1927, The University of Texas Southwestern Medical Center. **DECIPHERING THE GLUTAMINE SIGNALING PATHWAY TO mTORC1.**

In Aims 1 and 2 we generated multiple tools (plasmids and CRISPR/Cas9 knockout (KO) and knock-in cell lines) in order to better understand roles of ArfGAP1 and SNAT7 in glutamine signaling to mTORC1. In Aim1 we generated Arf1GAP1 knockout (KO) cell lines and made stably HA- tagged ArfGAP1 cells that we used for immunoprecipitation and subsequent mass spectrometry (IP-MS) experiments (Aims 1 & 3). In Aim 2 we made SNAT7 KO cell lines and generated a HA-tagged SNAT7 cell line that we used for IP-MS experiments (Aims 2 & 3). Currently, we are analyzing the IP- MS results and validating novel interacting proteins for ArfGAP1 and SNAT7. Potential interacting proteins will be confirmed by co-immunoprecipitation experiments. After validation, the interacting proteins will be knocked out using CRISPR/Cas9 genome editing. The KO cells will be analyzed for mTORC1 activity under a variety of different conditions (normal culturing conditions, amino acid starvation, and glutamine stimulation). We anticipate we will discover novel ArfGAP1 and SNAT7 interacting proteins that regulate mTORC1 activity in response to glutamine levels.

In Aim 3, we utilized an endogenously tagged Raptor-GFP (Raptor is a component of mTORC1) HAP1 cell line and performed IP-MS experiments under different conditions. We have found approximately 14 Raptor-GFP interacting proteins that only interacted with Raptor under a specific condition. We have validated 6 of them by co-immunoprecipitation experiments, and we are investigating if these proteins play a role in glutamine signaling to mTORC1. Initially, we will KO these Raptor interacting proteins and determine whether or not they play a role in modulating mTORC1 activity in response to glutamine. We anticipate that these Raptor interacting proteins will play a role in glutamine-induced mTORC1 activation. We believe that this is an important area of research in cancer biology that may lead to treatments for human cancers.

JEAN X. JIANG, AQ-1507, The University of Texas Health Science Center at San Antonio. **MODULATING HEMICHANNEL ACTIVITIES USING TARGETING ANTIBODIES.**

Two monoclonal antibodies, M1 and M2 both target to extracellular E2 domain of Cx43 protein. However, M1 antibody blocks while M2 antibody activates Cx43 hemichannel activity. In this study period, we tested several biophysical properties of these two antibodies; 1. Stability of these two antibodies the antibody ; 2. isolated Fab fragment antigen binding affinity. We have tested stabilities of these antibodies under higher temperature and different durations. The protein properties were measured by gel electrophoresis, turbidity/light scattering, sedimentation and surface plasma resonance. The antibodies are very stable and even after 14 days at 40oC, there was no detectable aggregation and protein degradation and binding affinity was preserved. The Fab fragment affinity assay was conducted using Biacore 3000 equipment in our Institutional Protein Interaction Core. Briefly, CM5 chips were coated with biotinylated peptide and then analytes, Fab fragments of M1 or M1 (antigens) was passed through to measure binding affinity in real time. Based on the kinetic parameters, we determined binding affinities of both Fab fragments were in the range of 10⁻⁷ to 10⁻⁸ M. These results suggest that these two antibodies were highly stable with high specificity based on Fab fragment binding assay.

JIN JIANG, I-1603, The University of Texas Southwestern Medical Center. **BIOCHEMICAL STUDY OF Hh SIGNALING AT THE PRIMARY CILIUM.**

Primary cilium, a microtubule-based plasma membrane protrusion found in most mammalian cells, regulates many essential cellular processes and its malfunction attributes to numerous human disorders collectively called ciliopathy. Primary cilia provide a special subcellular compartment for transducing extracellular signals, most notably, the Hedgehog (Hh) signal. Hh family of secreted proteins plays pivotal roles in both embryonic development and adult tissue homeostasis. Deregulation of Hh signaling activity has been linked to numerous human diseases including birth defect and cancer. The Hh signal is transduced by the GPCR family protein Smoothened (Smo) and the Zn-finger transcription factor Gli, both of which are localized at the primary cilium in response to Hh. However, how Smo transduces the Hh signal to activate Gli proteins at the primary remains poorly understood. We have identified conserved Ser residues in the N-terminal region of the Gli family of transcription factor (S218/S220 in Gli2) that are required for Gli activation. We have generated a phospho-specific antibody that recognizes phosphorylated S218/S220 (pS218/S220) in Gli2. We found that phosphorylation of S218/S220 was stimulated by Shh and required ciliary localization of Gli2. In *Drosophila*, Hh/Smo activates Ci (the *Drosophila* Gli protein) through the Ser/Thr kinase Fused (Fu). In mammals, there are two Fu homologs: ULK3 and STK36. To determine which kinase is involved in Gli2 phosphorylation, we used the CRISPR/Cas9 system to delete either ULK3, STK36, or both. We found that deletion of either ULK3 or STK36 reduced while their combined deletion nearly abolished Shh-stimulated phosphorylation of Gli2 as well as the expression of Hh target genes. Reintroducing either ULK3 or STK36 into the double mutant cells restored Gli2 phosphorylation and Hh target gene expression, suggesting that ULK3 and STK36 act redundantly to transduce the Hh signal from Smo to Gli proteins.

NING JIANG, F-1785, The University of Texas at Austin. **IDENTIFY THERAPEUTIC ANTIBODIES AND VACCINE CANDIDATES BY MINING HUMAN ANTIBODY REPERTOIRE IN MALARIA.**

During the third year of the award, we finished the antibody repertoire sequencing study in young children with malaria and the results were published on Nature Communication. We also developed a streamlined approach to predict and validate new antibody novel germline alleles. These results were published on Frontiers in Immunology.

At the same time, we collaborated with Laura Su at University of Pennsylvania to characterize follicular T cell repertoire in HIV positive individuals. We discovered antigen driven clonal expansion in these cells that was not known before. The manuscript describing these findings was in *Science Immunology*.

We also extended the immune repertoire sequencing to TCR and this technology development was published on *Frontiers in Immunology*.

In addition, we study the contribution of CD8 to different TCRs with different affinity and found that normalized synergy that predicts CD8 co-receptor contribution to TCR and pMHC binding decreases as TCR affinity increases in human viral-specific T cells, suggestion that TCRs with high affinity is truly independent of CD8 binding. These findings were published on *Frontier in Immunology*.

YOUXING JIANG, I-1578, The University of Texas Southwestern Medical Center. STRUCTURAL AND FUNCTIONAL STUDIES OF LIGAND-GATED CATION CHANNELS.

Over the past year, the Welch grant has been used to support the studies of several physiologically important ion channel proteins in cellular organelles. With the recent technology development in electron microscopy, we are taking single particle cryo-EM method as the main approach to obtaining the structures of these organellar channels.

(1). The transient receptor potential mucolipin 1 (TRPML1) is an endo/lysosomal cation channel ubiquitously expressed in mammalian cells and its loss-of-function mutations are the direct cause of Type IV mucopolidosis, an autosomal recessive lysosomal storage disease. We determined the EM structure of the mouse TRPML1 channel, providing structural insights into the PIP2 regulation as well as the luminal pH and calcium modulation of channel conduction in TRPML1.

(2). TRPM4 is a calcium-activated, PIP2 modulated, monovalent-selective cation channel, and belongs to the family of melastatin-related transient receptor potential (TRPM) channels. TRPM4 activation can depolarize the plasma membrane potential and activate voltage-gated sodium channels or calcium channels. Thus, its function has been implicated in many important physiological processes. We determined the EM structures of the mouse TRPM4 channel in the presence and absence of ATP, revealing the molecular architecture of the TRPM family for the first time.

(3). Mammalian TPC channels are localized to the endolysosomal membrane and their functions are associated with various physiological processes, such as hair pigmentation, mTOR-dependent nutrient sensing, lipid metabolism and Ebola virus infection. Following our previous study on plant TPC1, we recently determined the EM structures of mouse TPC1 in both open and closed states which, combined with functional analysis, provide comprehensive structural insights into the selectivity and gating mechanisms of mammalian TPC channels.

LUKASZ A. JOACHIMIAK, I-1928, The University of Texas Southwestern Medical Center. STRUCTURAL BASIS FOR CHAPERONE FUNCTION IN POLYGLUTAMINE AGGREGATION.

We applied integrative structural methods including XL-MS, ssNMR and crystallography to interrogate the DNAJB8 oligomer. First, using novel crosslinking chemistries developed in my lab we identified acid- lysine crosslinks including long-range contacts between the J-domain (JD) and C-terminal Domain (CTD) of DNAJB8, consistent with a possible interaction between these terminal domains. In collaboration with Dr. Van der Wel (University of Pittsburgh), we carried out ssNMR experiments to measure domain dynamics of the DNAJB8 and found that the oligomers are surprisingly rigid and that a subset of JD peaks are narrow possibly due to protein-protein contacts. Indeed, experiments in higher ionic strength abrogate long-range crosslinks and broaden ssNMR peaks. Ongoing biochemical and solution NMR experiments on isolated JD and CTD domains will validate this mode of interaction. We also asked how the disordered middle domains contribute to the oligomer. Computational methods predicted amyloidogenic regions and we designed peptides to probe aggregation propensity. We identified a 20- mer peptide that produces ThT signal and forms large structures by TEM. In collaboration with Dr. Eisenberg (UCLA), we determined a DNAJB8 fragment structure that shows a possible mechanism of oligomerization via a phenylalanine ladder. Mutagenesis of key sites in the peptide and in full-length protein alters oligomer assembly. These data support at least two mutually exclusive modes of interactions in the oligomer. We anticipate that a combined perturbation of these sites should interfere with oligomer formation and may play a role in substrate activity. Future work will extend these methods to study how DNAJB8 interacts with substrates. Our data support a topology for the DNAJB8 oligomer that differentially exposes surfaces for substrate interaction. In future experiments we anticipate testing the role of these mutants in aggregation suppression in cells.

KENNETH A. JOHNSON, F-1604, The University of Texas at Austin. DYNAMICS OF STRUCTURAL CHANGES GOVERNING DNA AND RNA REPLICATION.

Hepatitis C virus (HCV) inhibition Project: After overcoming some technical difficulties, we have nearly completed a study of 6 different nucleoside analogs, including the clinically important Sofosbuvir (from Gilead) that is used to treat HCV infections. One of the major challenges in designing an effective nucleoside analog to act as a chain terminator during polymerization is that HCV polymerase has a high rate of ATP-dependent excision of chain terminators. This activity, first discovered for mutant forms of HIV reverse transcriptase that are resistant to thymidine analogs, involves the reaction of ATP with the DNA primer strand to excise the 3'-terminal nucleotide forming a dinucleoside tetraphosphate. The rate of this reaction catalyzed by the HCV polymerase is 100-fold faster than that of the drug-resistant form of HIV reverse transcriptase. Our studies have revealed that Uridine nucleotides are particularly resistant to excision, explaining the clinical effectiveness of Sofosbuvir.

Artificial fluorescent amino acid project. We have succeeded in efficiently labeling a fast, high fidelity DNA polymerase with a fluorescent amino acid. The label has provided a signal to measure the rates of the conformational change after substrate binding. Remarkably, the rate of the conformational change is greater than 5000/s and is followed by a rate of chemistry of about 300/s. However, the rate of nucleotide escape before chemistry is only 1/s,

supporting our new paradigm for understanding the role of induced-fit as a major determinant of enzyme specificity. We have a large data set of equilibrium and kinetic data that we have fit globally to a single comprehensive model to define the full reaction free energy profile, including reversible chemistry, product release and DNA translocation. This will constitute the most comprehensive kinetic and thermodynamic analysis of and polymerase to date.

KEITH P. JOHNSTON, F-1319, The University of Texas at Austin. CONTROLLED ASSEMBLY OF INORGANIC AND ORGANIC NANOPARTICLE CLUSTERS.

Nanoparticle assemblies in water and at the water-air interface are being designed to produce ultra-stable air-in-water foams, by inducing interfacial viscoelasticity. To design these assemblies with the desired properties, the nanoparticle surface chemistry is being modified to control the interfacial interactions. As the elasticity increases, both the drainage of the lamellae films in the foam and the coarsening of the bubbles were arrested. In the case of gold nanoparticles, reversible self-assembly was tuned with pH to achieve self-limited growth with significant characteristics of equilibrium behavior, without cluster-cluster aggregation. For monoclonal antibodies (mAbs) at high concentration (up to 250 mg/mL), our ongoing studies of the nature of protein-protein interactions (PPI) and their effect on reversible self-association (clustering) are advancing the understanding protein stability and rheological properties. Cluster size distributions from coarse-grained simulations of small angle X-ray scattering data and light scattering are being related systematically to short-ranged attractive interactions at particular locations on the protein surfaces. Furthermore, these cluster size distributions are providing novel insight into the viscosities of the mAb solutions. In our electrochemical research, high surface area perovskite (and Ruddlesden-Popper) nanoparticle clusters were synthesized and utilized to catalyze the electrooxidation of urea, methanol and ethanol. By systematically increasing Ni – O bond covalency, the inherent oxidation state of Ni was extended past +3 to increase catalyst activity, indicating a governing principle for the rational catalyst design. Furthermore, we have controlled the nanoscale geometry of perovskite clusters and nitrogen- doped carbon nanotubes (N-CNT) to provide guidelines for increasing knowledge of activities in the oxygen evolution and oxygen reduction reactions.

RICHARD A. JONES, F-0816, The University of Texas at Austin. MOLECULAR PRECURSORS TO NEW FUNCTIONAL MATERIALS.

We have continued with our work on high nuclearity luminescent clusters of the lanthanides. In addition to the “nanodrums” formed with Cd²⁺ ions we have further explored systems with alternative d-block metals. With Zn²⁺ work with flexible long chain Schiff base ligands with linker groups featuring poly- ether (-CH₂)₂(-O-(CH₂)₂-O(CH₂)₂-) or amine (-CH₂)₂NH(CH₂-) functional groups has now been published. Three luminescent Zn–Ln clusters [Ln₈Zn₆(L₁)₂(OAc)₂₀(O)₂(NO₃)₄(OH)₄] (Ln = Sm (1) and Nd (2)) and [Nd₄Zn₄(L₂)₂(OAc)₁₀(NO₃)₂(OH)₄] (3) were prepared using these ligands. These clusters exhibit unusual nano-square-like structures, unlike the “nanodrums” previously reported. In other, now published work, four luminescent 32-metal Cd–Tb nanodrums, [Tb₈Cd₂₄(L₁)₁₂(OAc)₄₈] (4), [Tb₈Cd₂₄(L₂)₁₂(OAc)₄₈] (5), [Tb₈Cd₂₄(L₃)₁₂(OAc)₄₈] (6) and [Tb₈Cd₂₄(L₂)₁₂(1,4-BDC)₄(OAc)₃₈(OH)₂] (7), were constructed from three specially designed chain-like Schiff base ligands H₂L_{1–3} with flexible carbon–carbon backbones containing 5, 6 and 10 methylene units, respectively. In addition to the Schiff base ligands (the primary energy transfer donors), four 1,4-BDC bridging units were successfully introduced into the structure of 7. In addition to providing increased structural stability, the 1,4-BDC units act as secondary energy transfer donors providing extra energy for lanthanide luminescence, which results in improved luminescence properties when compared to those of the related Cd–Ln nanoclusters without 1,4-BDC units. In vitro investigations on 7 with SGC and PANC cancer cells revealed an accumulation of the molecular nanoparticles in the cells, as confirmed by confocal microscopy. The cytotoxicity of 7 toward the SGC and PANC cells is moderate (IC₅₀ values of 7 lie in the range of 15–60 mM). ICP-MS analysis reveals that cellular uptakes of 7 in 1000 SGC and PANC cells after treatment for 3 hours are 0.0094 pmol and 0.015 pmol, respectively.

MIGUEL JOSE YACAMAN, AX-1615, The University of Texas at San Antonio. DESIGNING HIGHLY ACTIVE NOBLE METAL CATALYSTS USING Ni, Co AND Cu: A NEW GENERATION OF CATALYST.

My research team has been successful in meeting our research objectives. Specifically, we performed studies to decipher the oxygen reduction reaction (ORR) catalytic activities of diverse architectures on graphene derived from reduced graphene oxide. We found that the mechanistic origin of ORR activity is associated with the trace manganese content and reaches its highest performance at an onset potential of 0.94V when manganese exists as a mononuclear-centered structure within defective graphene. These studies exposed the deceptive role of trace metal in formerly thought to be metal-free graphene materials and provided insight into the design of better-performing catalyst for ORR by underscoring the coordination chemistry possible for future single-atom catalyst materials.

Additionally, we performed studies regarding the effects of Argon (Ar⁺) ion bombardment of crystalline diamond, polycrystalline diamond films, and graphite, as reference, on the BE position of the C 1s XPS peak arising from the XPS analysis of these materials. These studies showed that 1) Ar⁺ ion bombardment is a reliable technique to characterize Diamond vs graphite materials during XPS analysis; 2) A low energy peak reported as C 1s/sp² bonding, is attributed to the C 1s/sp³ in the presence of Ar atoms inserted in the lattice. 3) The data show direct correlation between the energy of the Ar⁺ ion beam used for surface sputter-cleaning and binding energy shifts of XPS C 1s peaks. Further analysis may provide information about the position of Ar atoms in the diamond lattice to identify what potential beneficial or deleterious effects may be deduced from the interaction of Ar atoms with the lattice of diamond-based materials. Atoms implantation in Diamond using a low energy beam could be a new way to manufacture doped diamond nano-devices for nano-electronics, NEMS and MEMS, and others diamond-based devices. These studies and their implications are detailed in the publications.

KARL M. KADISH, E-0680, University of Houston. ELECTROCHEMISTRY AND SPECTROELECTROCHEMISTRY OF COMPOUNDS WITH MULTIPLE REDOX CENTERS.

Our research during the last year focused in large part on four types of compounds: (1) tetrapyrroles with highly substituted porphyrin, corrole or porphyrazine skeletal structures, (2) phthalocyanines and subphthalocyanines, (3) transition metal bis(phenolate)dipyrins and (4) dipyrromethenes (BODIPYS).

Some of the examined compounds contained multiple fused ring systems, some contained multiple electron-withdrawing or p-extending substituents and some contained multiple redox active groups such as ferrocene, substituted nitrobenzene or N-methylbenzene. One overall goal of our research is to unify descriptions of porphyrin and phthalocyanine electrochemistry with that of related hybrid macrocycles while also improving our ability to predict and tune redox activity for applications in a variety of areas. Some achievements in this area were highlighted in a 2017 Chem Review article on metallocorroles and others will appear in a major metalloporphyrin review to be submitted before the end of 2018. During the last grant year we continued to characterize previously unknown transition metal porphyrins in both high and low oxidation states while also turning our attention to the electrosynthesis of new metallomacrocycles which were either isolated for further study or in-situ generated and characterized by a variety of spectroscopic techniques. Finally, we continued to expand the known redox chemistry of porphyrins, corroles and phthalocyanines while concentrating on reactions previously not observed within the potential window of the electrochemical solvent but readily accessible in the following ways: (1) by synthesis of new derivatives with very specific substituents at the meso and/or β -pyrrole positions of the macrocycle, (2) by introduction of specific axial ligands or other molecules to solution and/or (3) by judicious use of variable and low temperature electrochemistry to best evaluate and control the presence of previously unknown coupled chemical reactions.

CRAIG D. KAPLAN, A-1763, Texas A&M University. FUNDAMENTAL MECHANISMS OF RNA POLYMERASE II TRANSCRIPTION.

Our Objective 1 progress is as follows: We have previously completed genetic screens for substitutions in TFIIF components Tfb3 and Ssl2 that alter transcription start site usage in vivo, in budding yeast. We now find that genetic interaction and molecular evidence are consistent with Ssl2 mutants altering processivity of promoter scanning – that is, how far the pre-initiation complex (PIC) may look downstream of the assembly site for start sites. Examination of mutant locations on a recent Cryo-EM structure of the PIC indicates the locations of different phenotypic classes of mutants are distinct, with presumptive reduced processivity substitutions distributed throughout the Ssl2 structure, as predicted for reduced function mutants. Intriguingly, the N-terminal domain of Ssl2 is not observed in the structure but contains both gain of processivity and loss of processivity substitutions. This domain appears to be a flexible regulatory domain possibly targeted by other flexible or unobserved residues within the PIC, validating the need to go beyond the structure for functional understanding. We are now generating genome wide data on ssl2 mutant effects on initiation, and have found that ssl2 mutants alter initiation at essentially all yeast Pol II promoters. We have undertaken now a screen for TFIIE initiation mutants, and we have at least two classes of mutant, each predicted to alter initiation in distinct ways. Objective 2 progress: we have constructed yeast promoter libraries comprising >40,000 promoter variants and are now using deep sequencing to quantify the output of each variant, to determine the sequence specificity of Pol II initiation. Finally, we have determined that Pol II mutants alter cell size in correlation with the extent of their transcription defects. We are pursuing the idea that cell size is not just a determinant of transcription and mRNA decay rate (previously proposed), but that cell size is responsive to transcription and mRNA decay rates.

ADRIAN T. KEATINGE-CLAY, F-1712, The University of Texas at Austin. PREPARATIVE BIOCATALYTIC SYNTHESIS OF COMPLEX POLYKETIDES.

Our lab has led a revolution in the understanding of a polyketide synthase module that nicely bridges the aims of this funding cycle with that of the next funding cycle. Our detailed analysis of the modules from all of the characterized trans-acyltransferase polyketide synthases (Vander Wood & Keatinge-Clay, 2018) firmly establishes that the module boundaries of all modular polyketide synthases begin and end at the C-terminal end of the ketosynthase domain, not at the N-terminal end as believed for the past three decades. Beyond nomenclature, this analysis impacts our understanding of module function, the evolution of assembly lines, pathway prediction, and assembly line engineering. We have already begun experiments to re-engineer the macrolactin polyketide synthase using this information. Our lab has continued to explore polyketide synthase enzymes that perform useful chemistry. We reported our structure/function studies of a pyran synthase from the sorangicin assembly line that cyclizes polyketide intermediates during assembly line synthesis (Wagner et al., 2018). By next week we will submit our structure/function studies on a gem-dimethylating methyltransferase from the disorazol assembly line. Our collaborator, Jianting Zheng (former postdoc), also worked with us to obtain the structure of a ketoreductase bound to a polyketide substrate (Liu et al., 2018) that provides much needed information for how ketoreductases enforce stereocontrol. We have also completed the chemoenzymatic synthesis of a library of two-stereocenter triketides that will be submitted shortly.

BEN KEITZ, F-1929, The University of Texas at Austin. PEPTIDE DIRECTED SYNTHESIS OF METAL-ORGANIC FRAMEWORKS.

We identified peptide sequences that bind to metal-organic framework surfaces via phage display. We visualized peptide binding through fluorescence microscopy and showed that it could influence drug delivery applications by improving MOF stability. We are now determining if these peptides can control MOF synthesis and crystallinity. In other work, we showed that an electroactive bacterium, *S. oneidensis*, can use MOFs as terminal electron acceptors. We also showed that this resulted in the synergistic removal of toxic Cr(VI) from solution. Similarly, we showed that electron transfer from *S. oneidensis* can control the formation of palladium nanoparticles. Finally, we showed that *S. oneidensis* can control extracellular redox-driven catalytic cycles through biological electron transfer. Specifically, we showed that bacterial metabolism can be used to control atom-transfer radical polymerization and synthesize polymers with well-defined molecular weights. Our work suggests that electroactive bacteria can be used to control a wide variety of abiotic

reactions through the mechanism of biological electron transfer. Overall, our work resulted in two accepted publications, with two more under review after uploading to the bioRxiv preprint server.

CHING-HWA KIANG, C-1632, Rice University. SINGLE MOLECULE AND SINGLE CELL STUDIES OF BIOLOGICAL SYSTEMS.

Studying the thermodynamics and mechanics of biological macromolecules through single molecule and single cell AFM force studies allowed us to gain detailed understanding of the intra- and inter-molecular interactions through force response. Protein activation often involves conformational transitions, and such switches are often difficult to characterize in multi-domain proteins. Full-length factor H (FH), consisting of 20 small consensus repeat domains, and some forms of FH can reduce the disulfide bonds linking large VWF multimers into smaller less adhesive forms. Other forms, such as the commercial purified factor H (pFH) has little or no vWF reductase activity unless the pFH is chemically modified by either EDTA or urea. We used atomic force microscopy (AFM) single molecule force measurements to investigate different forms of FH including recombinant factor H (rFH) and pFH in the presence or absence of EDTA and urea, and to correlate the conformational changes to its activities. We found that the VWF reductase activity of FH forms is dependent on FH conformation and on free thiol exposure. We have investigated the force response of single cells on different substrates and under other chemical compounds, and found that the step force of stretching cells increases as a function of the substrate stiffness, and can be changed under the influence with other chemicals. Furthermore, we have reviewed about observing dynamic states of single molecule DNA and proteins using AFM. Since force plays a fundamental role in many, if not all, biological systems, one way to reveal the dynamics of the molecules is to elucidate its intra- and inter-molecular force, which can be used as a marker to capture information about their conformational changes.

THOMAS C. KILLIAN, C-1844, Rice University. PUMP-PROBE SPECTROSCOPY OF RYDBERG-MACROMOLECULE DECAY PATHWAYS.

The first year of the grant has been extremely productive. We published results in Physical Review Letters and Physical Review A on production of Rydberg molecules in a dense background of ultracold strontium atoms. The density is ten orders of magnitude less than atmospheric density, but this yields hundreds of background atoms within the Rydberg electronic wave function, which is dense in the context of this experiment. Working with theory collaborators at Harvard and the Vienna University of Technology, we deciphered the photoexcitation spectrum for Rydberg molecules. The spectrum provides a measure of the background density in which the excitation takes place, which is valuable for studies of inelastic molecular collision rates. We also found that the Rydberg excitation, when viewed as an impurity in the quantum gas, severely perturbs the background density, connecting Rydberg molecules to the phenomenon of polarons in condensed matter systems.

We also published measurement of the lifetime of Rydberg molecules in the dense gas in Physical Review A and the Journal of Physics: Conference Series accompanying the International Conference in Photonic, Electronic, and Atomic Collisions. We extracted some information on the state-changing processes molecules undergo during the decay process and proposed a new model for the decay, which highlighted the overlap of the Rydberg electron with the Rydberg nucleus. Experiments in our laboratory have been at relatively low principal quantum number so far. We recently completed improvements on the apparatus that will allow us to study up to principal quantum number $n \sim 180$ in order to confirm scaling laws predicted in the model. We have also designed and will soon start constructing the millimeter-wave system that will allow us to study vibrational wave-packet dynamics as described in the proposal.

NAYUN KIM, AU-1875, The University of Texas Health Science Center at Houston. LOCUS-SPECIFIC QUANTITATION OF URACIL ASSOCIATED WITH UNSCHEDULED DNA SYNTHESIS.

This year, in order to determine whether the uracil-associated mutations at highly transcribed genes are affected by the change in the efficiency of uracil-AP turnover, we used a genetically engineered form of DNA glycosylase (CDG) that excises undamaged cytosines in addition uracil. The expression of CDG elevated uracil-dependent or cytosine-dependent mutations by ~ 10 -fold or ~ 2 -fold, respectively, indicating that the transcriptional effect on efficiency of the glycosylase is only a minor contributing factor in the transcription-dependent elevation in the uracil-associated mutations. And in further support of our proposed model where the correlation between active transcription and elevated uracil can be explained by the extensive repair-dependent DNA synthesis (i.e. UDS) at the highly transcribed genomic loci, we demonstrated that overexpression of dUTPase Dut1 in G1 and G2 phase of the cell cycle leads to a significant reduction in the uracil-dependent mutations in a transcription-dependent manner. Overexpression of Dut1 in S phase of the cell cycle had relative less effect on these types of mutations. A manuscript describing our model of UDS-dependent uracil incorporation into DNA and the supporting data was recently accepted and published in the journal PLoS Genetics.

We also made a significant progress in determining the role of AP endonuclease Apn2 in the excision repair of uracil-derived AP sites. We found that the repair of uracil-derived AP sites depends on whether the yeast cells are growing via respiration or fermentation and showed that the disruption of Apn2 results in significant reduction in the uracil-associated mutation specifically during respiratory growth. We are currently investigating whether the catalytic activity of Apn2 is necessary for this role in uracil-induced mutations and how the expression and/or post-translational modification of Apn2 are differentially regulated during respiratory and fermentative growth.

NATASHA KIRIENKO, C-1930, Rice University. STRUCTURAL DETERMINANTS OF PYOVERDINE CHEMICAL FUNCTION.

During Year 1 of my Welch Award, we have achieved progress toward both Aims of our proposal. For Aim 1, we developed an elaborate pyoverdine purification pipeline consisting of the following steps: 1) producing the material via bacterial growth; 2) centrifugation, filtration, and autoclaving

to remove bacteria and denature polypeptides; 3) reverse phase chromatography over C18 column; 4) removal of polypeptides >3 kDa via filtration; 5) final purification by HPLC; 6) dialysis; and 7) concentration.

Using this protocol, we purified two classes of pyoverdine produced by *P. aeruginosa* strain PA14, E1 and E2. E2 has increased hydrophobicity (it elutes at 75% methanol, while E1 elutes at 50%). We have also purified E1 and E2 equivalents from *P. aeruginosa* strain PAO1. The E1 structure for this strain is known and will be used as a reference point for validating further work. In Year 2 we will determine the structures of these four samples using mass-spectrometry and NMR.

For Aim 2, we have begun to analyze the biological properties of E1 and E2 from *P. aeruginosa* PA14 using two host models: the nematode *Caenorhabditis elegans* and mammalian macrophage cell lines. Unexpectedly, only E2 (but not E1) impairs Complex I of the ETC in mitochondria (shown by increased NADH/NAD⁺ ratio), resulting in the autophagic degradation of this organelle (shown by stabilization of the kinase PINK-1/PINK1, targeting of mitochondria to autophagolysosomes for degradation, decreased mitochondrial DNA, and a strong drop in ATP production). Our experiments with macrophages suggest that both E1 and E2 enter cells, albeit via different mechanisms. E1 is largely endocytosed and localizes to punctae, which are possibly lysosomal vesicles. E2, in contrast, is diffusely distributed in the cytoplasm. The mechanism of E1 endocytosis, the identity of the subcellular compartment that contains E1, and the mechanism of E2 translocation are subjects of ongoing research.

STEVEN A. KLIEWER, I-1558, The University of Texas Southwestern Medical Center. **MECHANISMS UNDERLYING THE SECRETORY ACTIONS OF FGF21 IN EXOCRINE PANCREAS.**

The nuclear receptor, peroxisome proliferator-activated receptor-gamma (PPAR-gamma), is a master regulator of adipocyte differentiation and the target for the insulin-sensitizing thiazolidinedione (TZD) drugs used to treat type 2 diabetes. In cell-based *in vitro* studies, the transcriptional activity of PPAR-gamma is inhibited by SUMOylation at K107 in its N-terminus. However whether this post-translational modification is relevant *in vivo* had remained unclear. This past year, using mice homozygous for a mutation (K107R) that prevents SUMOylation at this position, we demonstrated unequivocally that PPAR-gamma is SUMOylated at K107 in both visceral and subcutaneous white adipose tissue. We further showed that in the context of diet-induced obesity, PPAR-gamma-K107R mutant mice have enhanced insulin sensitivity without the corresponding increase in adiposity that typically accompanies PPAR-gamma activation by TZDs. Accordingly, the PPAR-gamma-K107R mutation had no effect on adipocyte differentiation *in vitro*. We conclude that PPAR-gamma SUMOylation at K107 is physiologically relevant and may serve as a pharmacologic target for uncoupling PPAR-gamma's beneficial insulin-sensitizing effect from its adverse weight gain. We are currently comparing the genes and biological pathways regulated by the K107R mutation, the TZD diabetes drug rosiglitazone, and the two together in white adipose tissue. We anticipate that these studies will provide new insights into the physiologic and pharmacologic actions of PPAR-gamma.

CHE MING KO, A-1358, Texas A&M University. **THEORETICAL STUDIES OF HEAVY ION COLLISIONS.**

We have continued to improve the relativistic transport model for heavy ion collisions at intermediate energies, particularly the treatment of the collision term in the presence of mean-field potentials. Using this model, we have studied the influence of pion in-medium effects on the ratio of produced charged pions. For heavy ion collisions at relativistic energies, we have studied light nuclei production based on the coalescence model and showed that the ratio of the product of triton and proton yields to the square of the deuteron yield depends on the neutron density fluctuation at kinetic freeze-out. A peak is found from the experimentally measured ratio at a collision energy where a large density fluctuation is expected from the critical transition of produced quark matter to a hadronic matter. We have also used the coalescence model to study hypertriton production in relativistic heavy ion collisions and found that because of its small binding energy and large size, hyperon triton is produced significantly later after the kinetic freeze-out of nucleons. For non-central heavy ion collisions at relativistic energies, we have found via the chiral kinetic theory, which takes into account the interplay between nearly massless quarks with their intrinsic spins, that the large vorticity field generated during the collisions can lead to the spin polarization of quarks, whose coalescence results in lambda hyperons with their polarizations consistent with experimentally measured values. Based on the chiral kinetic theory, we have also studied the effect of magnetic field generated in non-central heavy ion collisions on the separation of positive and negative charges relative to the reaction plane in collisions of isobaric systems, which have same atomic but different proton numbers, and found that the effect could be measurable only if the lifetime of the magnetic field is sufficiently long.

JENNIFER J. KOHLER, I-1686, The University of Texas Southwestern Medical Center. **DISCOVERING THE GLYCOCONJUGATE OF PERTUSSIS TOXIN.**

We have worked to identify host cell glycoconjugates recognized by two bacterial toxins – cholera toxin (CT) and pertussis toxin (PT).

In collaboration with the Yrlid lab (University of Gothenburg, Sweden), we examined CT binding to primary human and murine cells from blood and small intestine. We found that the fucosylated LewisX glycan was an important contributor to toxin binding. Moreover, mice deficient in the canonical cholera toxin receptor (GM1) remained susceptible to CT, demonstrating that host GM1 is not required for CT-induced diarrhea. This work was published in *PLoS Pathogens*.

We used competition binding assays to decipher the molecular determinants for fucose inhibition of CT binding. Human milk oligosaccharides (HMOs) and the LeY tetrasaccharide were able to inhibit CT binding to both intestinal epithelial cell lines and human primary intestinal epithelial cells. In collaboration with the Sampson lab (Stony Brook University), a non-natural fucose-containing polymer was shown to potently inhibit CT binding. This work was published in *ACS Infectious Diseases*.

We used small molecule inhibitors of glycosylation to discover the classes of host glycans recognized by PT, revealing a reliance on N-linked and sialylated structures. Additionally, host fucosylation protects cells against PT binding. We have also isolated host glycoproteins that interact directly with PT, and validation of these putative receptors is in progress.

We also used a photocrosslinking N-acetylglucosamine (GlcNAc) analog developed in this lab to discover human proteins that recognize the O-GlcNAc intracellular post-translational modification. In collaboration with the Boyce lab (Duke University), we found that 14-3-3 proteins can recognize O-GlcNAcylated proteins in vitro and in cells. The three-dimensional structure of a complex between a 14-3-3 protein and an O-GlcNAcylated peptide was determined. This work was published in Proc. Natl. Acad. Sci. U. S. A.

ANATOLY B. KOLOMEISKY, C-1559, Rice University. UNRAVELING THE CHEMICAL MECHANISMS OF SELECTIVITY IN CHANNEL-FACILITATED MOLECULAR TRANSPORT.

We presented a quantitative theoretical approach to analyze the mechanisms of genome interrogation by CRISPR RNA-protein complexes, which consists of searching for the target and selective cleavage of nucleic acids at specific locations. Theoretical method is based on the discrete-state stochastic description of the system that takes into account the most relevant physical-chemical processes. It is found that the target location is a two-state process, and the search dynamics is strongly affected by off-target cutting. Theoretical calculations explain well the available experimental observations, and give several testable predictions.

We also developed a new theoretical framework to describe the distributions of dynamic properties of biological molecular motors. It is based on the method of first-passage processes. The method was applied for analyzing the distributions of run lengths of motor proteins moving along linear filaments. It is found that these distributions are affected by the finite length of linear tracks, by the initial of the motor proteins along the filament and by the intermediate chemical transitions during the enzymatic cycle of motor proteins. These observations allowed us to clarify the chemical mechanisms of motor proteins functioning.

In addition, we investigated the mechanisms of chemical and biological processes that involve alternating dynamics by considering a dynamic search process of finding a small target on a 2D surface if the participating molecules can switch between the surface and bulk solutions. Both continuum and discrete-state stochastic descriptions are presented, and it is shown that there are significant differences between predictions of both methods. It is found also that the system can exhibit 3 different search regimes, which are determined by the size of the area visited by the molecule during one search cycle. Furthermore, search dynamics is sensitive to the location of the target in some dynamic regimes.

JUNICHI KONO, C-1509, Rice University. OPTICAL, INFRARED, AND TERAHERTZ SPECTROSCOPY OF LOW-DIMENSIONAL MATERIALS.

During the last year, we made progress in three different projects. First, we developed a unique architecture in which excitons in an aligned single-chirality carbon nanotube film interact with cavity photons in polarization-dependent manners. The system reveals ultrastrong light-matter coupling for polarization parallel to the nanotube axis, whereas coupling is absent for perpendicular polarization. Between these two extremes, the coupling strength is continuously tunable through polarization rotation with exceptional points separating crossing and anticrossing. The demonstrated on-demand ultrastrong coupling provides ways to explore topological properties of polaritons and quantum technology applications. Second, we made the first observation of intersubband plasmons in carbon nanotubes. The plasmon peak appeared in gated films of aligned single-wall carbon nanotubes only for probe light polarized perpendicular to the nanotube axis and only when carriers are present either in the conduction or valence band. Both the intensity and frequency of the peak were found to increase with the carrier density, consistent with the plasmonic nature of the resonance. Finally, we fabricated a weaved, substrateless, and polarization-sensitive photodetector based on doping-engineered fibers of highly aligned carbon nanotubes. This room-temperature-operating, self-powered detector responds to radiation in an ultrabroad spectral range, from the ultraviolet to the terahertz, through the photothermoelectric effect, with a low noise-equivalent power (a few nW/Hz^{1/2}) throughout the range and with a ZT-factor value that is twice as large as that of previously reported carbon nanotube-based photothermoelectric photodetector.

BRIAN A. KORGEL, F-1464, The University of Texas at Austin. NANOMATERIALS ASSEMBLIES.

Silicon (Si) nanocrystals were examined in biological systems to determine their interactions with living cells and their potential usefulness as imaging contrast agents for disease detection. Si nanocrystals are biocompatible and have fluorescence lifetimes on the order of 10's of microseconds making them candidates for imaging techniques that make use of the fluorescence lifetime. Si nanocrystals were tested as fluorescence contrast agents for biological imaging using two-photon excitation and fluorescence lifetime imaging microscopy (FLIM) for multiplex biological imaging in conjunction with fluorescent dyes that emit in the same spectral region (e.g. 600-700 nm), but with short lifetime signals (~ 2-5 ns, fluorescent dye). This technique, referred to as time-gated imaging, could be used to eliminate the autofluorescent background of cell tissue as well, for higher resolution, higher-precision imaging. Using a single two-photon excitation source at 800 nm, the fluorescence from two dyes (one blue emitting and one red emitting) and Si nanocrystals was measured simultaneously and spectral, as well as temporal, multiplexing was used to visualize the localization of the imaging contrast agents within the cells. This technique was used with various organelle dyes to observe the colocalization of Si nanocrystals in the endosomes of mouse macrophage cells. In another line of research, luminescent CH₃NH₃PbI₃ nanocrystals with cuboidal shape and tetragonal crystal structure were synthesized with high uniformity and assembled into superlattices. The nanocrystals were terminated by (110) and (002) facets, based on grazing-incidence wide-angle scattering (GIWAXS) and atomic

structure model. The assemblies were heated with in situ GIWAXS and grazing incidence small angle X-ray scattering (GISAXS) and transitions from tetragonal to cubic $\text{CH}_3\text{NH}_3\text{PbI}_3$ was observed with the subsequent degradation into hexagonal PbI_2 and rhombohedral PbI_2 .

LÁSZLÓ KÜRTI, I-1764, The University of Texas Southwestern Medical Center. NEW PARADIGMS IN HETEROCYCLIC CHEMISTRY.

During the first year of the new grant period the majority of efforts have been directed on the development of new reagents that allow the rapid synthesis of structurally diverse heterocycles. We found that soft C-nucleophiles (i.e., enolates) derived from ketones, nitriles and alpha-halogenated esters exclusively add to the carbon atom of the C=N bond in N-aryl iminomalones. This is in sharp contrast with the high N-selectivity observed during the addition of hard C-nucleophiles (i.e., aryl and heteroarylmetals). The new reactivity allowed the development of a general synthetic strategy for the preparation of 3-, 4-, 5- and 6-membered heterocyclic unnatural amino acid derivatives: (a) fully substituted aziridines were obtained in a single step when enolates of alpha-bromo esters were employed as nucleophiles; (b) enantiomerically enriched azetidines, gamma-lactones and tetrahydroquinolines were obtained via a two-step catalytic asymmetric reduction and cyclization sequence from adducts derived from ketone enolates and (c) highly-substituted gamma-lactams were prepared in one-pot from adducts obtained using acetonitrile-derived nucleophiles. We will continue to explore the reactivity of N-substituted iminomalones with other soft C-nucleophiles, especially catalytic asymmetric processes. We have also developed an efficient Cu(I)-catalyzed method for the synthesis of sterically congested ethers and thioethers from alpha-bromo carbonyl compounds and corresponding nucleophiles. This scalable transformation proceeds at ambient temperature and is tolerant towards air and moisture. We anticipate that this method will benefit the field of medicinal chemistry and chemical biology, where hindered ethers are commonly found as structural motifs in biologically-active molecules and small molecule probes, yet no general synthetic tools have been available for their synthesis. Currently studies are underway to further probe the reaction mechanism and expand the reaction scope.

JAAN LAANE, A-0396, Texas A&M University. MOLECULAR STRUCTURES AND VIBRATIONAL POTENTIAL ENERGY SURFACES IN GROUND AND EXCITED ELECTRONIC STATES.

Spectroscopic investigations of molecular structures, conformations, bonding interactions, and potential energy surfaces in ground and excited electronic states have continued utilizing both experimental and theoretical methods. Vibrational spectroscopy (infrared and Raman) has been utilized to study the electronic ground states while electronic spectroscopy in the ultraviolet region provides data on electronic excited state structures and vibrations. Theoretical ab initio and density functional theory (DFT) computations were used to complement the experimental work. The work on the theoretical potential energy surfaces (PESs) for bicyclo[3.1.0]hexane and four related molecules has been accepted for publication. The PESs were computed and these were found to be in excellent agreement with those determined from low-frequency infrared and Raman data. Calculations have also been completed on the PESs for cyclobutane and twenty-one related molecules and these also agree remarkably well with experimental results especially after the reduced mass models were refined. Infrared and Raman studies are far along on 2-cyclopenten-1-ol and two other molecules with intramolecular pi-type hydrogen bonding between pi systems and OH groups. Four molecules, including 3-cyclopenten-1-amine, possess interaction between pi systems and NH₂ groups. In each case the predicted conformations can be observed spectroscopically and the conformer with the pi bonding is the one of lowest energy. The theoretically predicted frequency differences for the conformations agree very well with those observed. Potential energy surfaces for these molecules have also been generated. The PESs for the internal rotations of 3-cyclopropen-1-ol and 3-cyclopropen-1-amine have also been determined and the results again show that the conformers with the pi-type hydrogen bonding are lowest in energy. Work is also continuing on the ground and excited states of substituted pyridines.

KEJI LAI, F-1814, The University of Texas at Austin. NONINVASIVE ELECTRICAL MAPPING OF CHEMICAL PROCESSES IN 2D MATERIALS.

In the past grant year, three papers supported by the PI's Welch award were published in high-impact journals. The PI is the corresponding author of all three works.

1. We have successfully synthesized monolayer $\text{WS}_2/\text{WS}_2(1-x)\text{Se}_2x/\text{WS}_2$ multi-junction lateral heterostructure via direct growth by chemical vapor deposition. We show that the local photoconductivity in the alloy region can be enhanced by two orders of magnitude over pure WS_2 due to carrier confinement. The paper was published and featured as the frontispiece in *Advanced Materials*.

2. We report the first quantitative nanoscale photoconductivity imaging on solar cell thin films by light-stimulated MIM. As visualized by the spatial evolution of local photoconductivity, the material degradation due to reaction with water that diffuses through the capping layer begins with the disintegration of large grains rather than the nucleation and propagation from grain boundaries. The work was published in *Nature Communications*. It was also reported as a news release in the National Renewable Energy Laboratory website see detail at website address listed below: (https://www.nrel.gov/news/press/2018/nrel_ut_scientists_discover_critical_factor_for_perovskite.html).

3. We have obtained few-layer In_2Se_3 flakes by mechanical exfoliation and vapor-phase deposition. Out-of-plane piezoelectricity and ferroelectricity are confirmed in these materials by confirmed by scanning transmission electron microscopy, second-harmonic generation, and Raman spectroscopy, and piezo-force microscopy measurements. The work shows the great potential of In_2Se_3 in electronic and photonic applications. The paper is now published in *Nano Letters*.

ALAN M. LAMBOWITZ, F-1607, The University of Texas at Austin. BACTERIAL REVERSE TRANSCRIPTASES: CHARACTERIZATION AND BIOTECHNOLOGICAL APPLICATIONS.

(1) Two papers listed as submitted in last year's Progress Report have now been published (Wu and Lambowitz 2017; Boivin et al. 2018). (2) In collaboration with Dr. Charles Thornton (U. Rochester), we developed methods for using thermostable group II intron RTs (TGIRTs) for analysis of RNAs containing GC-rich repeat expansions, which underlie the etiology of myotonic dystrophy, ALS, and other diseases, but are difficult to analyze by conventional method. (3) We published a first-of-its kind crystal structure of a full-length group II intron RT in ternary complex with template-primer substrate and incoming dNTP (Stamos et al. 2018). The structure revealed a host of novel features that contribute to the high fidelity and processivity of group II intron RTs, provided insights into how group II introns RTs function in RNA splicing and intron mobility, and revealed a remarkably close evolutionary relationship between group II intron RTs and RNA-dependent RNA polymerase. Going forward, this structure will enable comprehensive structure-function analysis and engineering of improved group II intron RTs for biotechnological applications. (4) We published a detailed characterization of the RNA splicing and mobility mechanisms of a *Geobacillus stearothermophilus* group IIC intron (denoted GsI-IIC), which has the unusual ability to proliferate to high copy number in its host genome and is the source of the thermostable group II intron RT (GsI-IIC RT), whose crystal structure we determined. Together with the crystal structure, this work establishes a comprehensive experimental system for studying the structural basis of group II intron splicing, mobility, and reverse transcription mechanisms (Mohr et al. 2018). (5) We continued to study free-standing bacterial RTs that are not associated with group II introns or other retroelements and obtained targeted gene distributions in a native host that will enable study of the physiological function of one of these RTs.

CHRISTY F. LANDES, C-1787, Rice University. IDENTIFYING HIDDEN CONFORMATIONS IN MULTI-STATE BIO-MOLECULES.

Over the past year, this project has come to completion. One of the project goals was to identify weakly stable intermediate states and to understand their role in biomolecular function. This past year, we developed a method to improve time resolution in single-molecule measurements, called Super-Temporal Resolved Microscopy (STRem). Because STRem can achieve over an order of magnitude faster time resolution compared to traditional camera resolutions, we used our new method to identify a previously unresolvable intermediate in protein adsorption/desorption equilibrium (Langmuir 2017, 33, 10818- 10828). We expect to be able to apply the STRem method in our new project. Another mechanistic issue addressed in the last year is that we require simultaneous space and time information in order to monitor fast non-equilibrium chemical processes. We developed, as part of a collaboration, a hyper-spectral microscope capable of imaging chemical dynamics with millisecond time resolution (J. Phys. Chem. C 2018, 122, 6865-6875). Finally, as part of our goal to address broad mechanistic questions, we quantified the role of allostery in a full neurotransmitter receptor with multiscale time and space dynamics (Nature Chem. Bio. 2017, 13, 1232-1238).

Additionally, we have gained exciting preliminary results towards a new direction - achieving a mechanistic description of chemical and biochemical separations. First, it has been suggested that rare events at a range of time scales contribute to decreased separations efficiency. We completed a preliminary study in which we showed the crucial role that polymer surface oxidation chemistry plays in either broadening or narrowing the dynamic range of protein surface interactions (Langmuir 2017, 33, 10818-10828). Next, because of our preliminary efforts on the long term project of achieving a mechanistic description of chromatography, we published an invited review (Ann. Rev. Phys. Chem. 2018, 69, 353-375).

OLEG V. LARIONOV, AX-1788, The University of Texas at San Antonio. NEW CATALYTIC STRATEGIES FOR THE SYNTHESIS OF COMPLEX HETEROCYCLES.

In this year we have focused on the development of novel reactions of nitroso compounds and the exploration of the synthetic scope and reactivity of these compounds. We continued to investigate the reaction of nitrogenous heterocycles with various organometallic reagents. We found that organosulfur nucleophiles can be used for nucleophilic substitutions of halogens in haloazines and their derivatives. Specifically, we found that the reaction is catalyzed by persulfates, and the reaction proceeds rapidly and can be completed in 15 min. The mechanism of the reaction was investigated and the crucial role of persulfate was discovered by NMR spectroscopy. Interestingly, although persulfate is mostly known as a radical initiator, we found that our reaction does not proceed by a radical mechanism. The reaction was further extended to the synthesis of symmetrical N-heterocyclic sulfides and sulfones. Further, we continued to study a simple and efficient method of synthesis of organoboron derivatives that we prepared for our investigation of the reactions of heterocyclic N-oxides with various carbon-centered nucleophiles. We developed preparative scale procedures that allow for aliphatic organoboron compounds to be readily synthesized from cyclohexenes in a photochemical reaction with trialkylboranes. The intermediate organoboron compounds can be used for the synthesis of five-membered carbocyclic and heterocyclic systems in a stereoselective manner. We have also studied the reactions of organosulfur nucleophiles in a palladium-catalyzed desulfurative coupling with haloazines and haloarenes. This study has led to the development of highly stereoselective formation of dienes from sulfinates. In conclusion, the year has led to a very productive expansion of our discoveries in the area of heterocyclic chemistry, and we are looking forward to accomplishing our research goals in the next year.

MICHAEL LATHAM, D-1876, Texas Tech University. METHYL-BASED NMR INVESTIGATION OF A DNA DOUBLE STRAND BREAK REPAIR COMPLEX.

In the last year, we have determined ideal DNA constructs for the DNA construct; however, the bulk of our work revolved around creating stable ATP-bound MR complex for NMR studies. Forming this ternary complex is problematic for several reasons, including hydrolysis of "non-hydrolysable" ATP analogs by Rad50 or breakdown of these analogs at the elevated temperatures where NMR studies are being performed and interference of transition state analogs with Mre11 activity. We are continuing to pursue different avenues to overcome this problem (e.g., mutations in Rad50 that do not hydrolyze ATP).

Moreover, we are continuing to refine our procedures for making higher concentrations of purified complex stable over longer periods of time. These advances will enable us to continue working toward our goal of a solution state structure.

The paper submitted during the last year, describing a dynamic allosteric network within Rad50 was published in Scientific Reports. Another paper related to our work from our Welch Foundation support will be published before the end of the summer. Moreover, graduate students supported by this grant have presented posters at the Southwest Regional American Chemical Society meeting and at the Texas Protein Folders and Function meeting.

SEONGMIN LEE, F-1741, The University of Texas at Austin. CHEMICAL, BIOCHEMICAL AND STRUCTURAL STUDIES OF INFLAMMATION-INDUCED DNA LESIONS.

During the 2017-2018 grant period, we have made significant progress toward achieving our proposed goals. Through the Welch-funded project, we have published one paper (Biochemical J) and submitted two additional papers (Nucleosides, Nucleotides and Nucleic Acids; Tetrahedron). One paper regarding 8-CIG is under preparation and will be submitted during the 2018-2019 grant period.

Aim 1.1. We have prepared 8-oxoA- and 8-CIG-containing DNA. In addition, we prepared 8-oxoinosine and 8-bromoadenosine phosphoramidites.

Aim 1.2. Using steady-state kinetics, we have determined kinetic parameters for DNA polymerases (beta and eta) replicating across 8-oxoA. Human DNA polymerase eta proficiently incorporated dGTP opposite 8-oxoA and extended dG:8-oxoA primer terminus, indicating that bypass of 8-oxoA by translesion DNA polymerases may be promutagenic. The minor groove interactions turned out to be important for the promutagenic replication.

Aim 2.1. To elucidate structural basis for DNA polymerase replicating across inflammation-induced DNA lesions, we determined three crystal structures of TLS DNA polymerase eta and three crystal structures of gap-filling DNA polymerase polβ in complex with templating 8-oxoA and 8-CIG. We also conducted mutation studies to gain insights into the factors contributing inflammation-induced mutagenesis. Aim 2.2. To assess the possibility of 8-oxoA-, 8-oxoG- and 8-CIG-induced interstrand cross-link (ICL) formation, we prepared duplex DNA containing 8-oxoA, 8-oxoG, 8-BrG, and 8-CIG. In the presence of hypochlorous acid and N-bromosuccinimide, the 8-oxoA-containing duplex DNA, but not DNA containing 8-oxoG, 8-CIG and 8-BrG, formed interstrand cross-links in good to high yields, indicating that inflammation can induce interstrand cross-links.

T. RANDALL LEE, E-1320, University of Houston. FUNCTIONALIZED XANTHATES, DITHIOLCARBOXYLATES, AND DITHIOLCARBAMATES FOR COATING SURFACES AND NANOPARTICLES.

In an invited feature article, we described the use of multidentate adsorbates for generating homogeneously mixed "conflicted" interfaces (Marquez et al. Langmuir 2017). Separately, we continued exploring the impact of headgroup architecture on film stability with a set of two aromatic-based bidentate adsorbates (Rittikulsittichai et al. Langmuir 2018). In other SAM-related work, we investigated transport properties of SAMs derived from partially fluorinated adsorbates bearing interfacial dipoles (Bruce et al. J. Phys. Chem. C 2018) and CN-terminated SAMs capable of resisting adhesion and adsorption of biological species (Park et al. AIMS Mater. Sci. 2018). Concurrently, we developed an inexpensive magnetoresistive sensor for the detection of biomolecules using magnetic nanoparticles (Qiu et al. Sens. Actuator A 2017). Moreover, we summarized efforts on the synthesis and use of bimetallic nanoparticles in biological applications (Srinoi et al. Appl. Sci. 2018) as well as the use of magnetic particles in biosensing techniques (Chen et al. Sensors 2017). We synthesized superparamagnetic nanochains with magneto-optical properties for use in biomedical detection applications (Vittur et al. Beilstein J. Nanotechnol. 2017), and magnetic nanocubes and nanospheres to determine the effect of shape on their sensing ability (Kolhatkar et al. ACS Omega 2017). Along these lines, we also probed the relationship between particle size and biosensing performance (Chen et al. Anal. Chem. 2018). We also synthesized temperature-responsive hydrogel-coated gold nanoshells conjugated with avidin that are suitable for targeted drug delivery (Park et al. Gels 2018). Also, we prepared anatase TiO₂ nanoparticles coated with partial gold shells for use in the photocatalytic generation of hydrogen via the splitting of water (Khantamat et al. J. Colloid Interface Sci. 2018).

GUGEN LI, D-1361, Texas Tech University. GROUP-ASSISTED PURIFICATION (GAP) CHEMISTRY FOR ASYMMETRIC SYNTHESIS AND CATALYSIS.

GAP chiral N-phosphonyl imines were found to be effective for the asymmetric reaction with azlactones [oxazol-5(4H)-ones] under mild and convenient conditions at room temperature. The reaction was conducted in the absence of any bases, additives and catalysts for a broad scope of substrate. Excellent chemical yields and diastereoselectivity have been achieved for more than thirty cases. The resulting α-quaternary syn-α,β-diamino acid products were purified simply by washing the crude mixtures with cosolvents without involving traditional chromatography or recrystallization methods. The auxiliary can be readily removed and recycled for reuse. GAP chiral N-phosphonyl imines were also utilized for the formation of N-phosphonyl β-enamino esters followed by the asymmetric reduction to give enantiopure β-amino esters/amides, which was controlled efficiently by using a combination of sodium cyanoborohydride and acetic acid. In the meanwhile, cobalt-catalyzed decarboxylative cross-coupling of (hetero)aryl carboxylic acids with benzothiazoles or benzoxazoles has been conducted. This work represents the first example of metal-catalyzed decarboxylative C-H heteroarylation of benzo-fused heterocycles, and provides a convenient system and approach to important arylheteroaryl and unsymmetrical biheteroaryl structural motifs with good yields and functional group tolerance. Finally, a novel [2+2] cycloaddition and 1,4-addition sequence induced by S-centered radicals was established by treating benzene-linked allene-ynes with aryldiazonium tetrafluoroborates and DABCO-bis(sulfur dioxide) in a one-pot system. The reaction provides a greener and more practical access to functionalized cyclobuta[a]naphthalen-4-ols with valuable applications. The reaction pathway is proposed to proceed by the following steps: [2+2] cycloaddition, insertion of SO₂, 1,4-addition, diazotization, and tautomerization, that were confirmed by parallel experiments.

PINGWEI LI, A-1931, Texas A&M University. THE STRUCTURAL BASIS OF RNA SYNTHESIS BY ZIKA VIRUS.

In order to obtain the crystals of ZIKV NS5 full-length protein in isolation or in complex with RNA or inhibitors, we need more NS5 proteins to screen and optimize the crystals. However, we could only get less than 1 mg ZIKV NS5 full length protein from 6L E.coli Rosetta (DE3) pLysS cells cultured in regular LB medium. In the past year, we tried many methods to optimize the conditions for NS5 protein expression, such as induction of E.coli cells with different temperature, different IPTG concentration, different cell density and different culture media. We also tried to optimize the conditions for NS5 protein purification, such as washing the Ni-column with different concentrations of imidazole. Finally, we found that we could get more than 3 mg pure ZIKV NS5 protein from 6L E.coli Rosetta (DE3) pLysS cells, which are cultured in Terrific Broth medium. The protein is as good as before and we could get the crystals in the same conditions. More proteins have facilitated us to screen and optimize the crystals.

We are optimizing the crystals of ZIKV NS5 protein in complex with a 17nt ssRNA by trying different buffers, changing the concentrations of salt and precipitant. In order to get the crystal of ZIKV NS5 protein in complex with RNA, we ordered two kinds of short single-strand RNA and mixed them with ZIKV NS5 or the RdRp domain for co-crystallization. We further mixed ZIKV NS5 protein or the RdRp domain, the short ssRNA and the nucleotide ATP or GTP to form a ternary complex and screened crystallization conditions. The soaking method was also used to get the crystals of the complexes.

We are screening and optimizing the crystals of ZIKV NS5 protein or the RdRp domain in complex with inhibitors. We have ordered two new inhibitors, Ribavirin and Sofosbuvir (R)-Phosphate. We mixed ZIKV NS5 protein or the RdRp domain with these two inhibitors for crystallization. We also mixed the ZIKV NS5 protein with inhibitors and short ssRNA together for co-crystallization.

WEI LI, C-1845, Rice University. EXOTIC COLLECTIVE PHENOMENA IN NUCLEAR CHEMISTRY AT A TRILLION DEGREES.

Highlights of achievements by the Rice high-energy nuclear physics group in the past year include the searches for anomalous chiral effects in nuclear collisions and first observation of collective phenomena of heavy mass quarks in proton-lead (pPb) collisions with the CMS experiment at the LHC. The group had a highly productive year, directly leading six publications as the principle author and contributing to more than 60 papers from CMS. The PI, Wei Li, and graduate student, Zhoudunming Tu, have pioneered a novel study of chiral magnetic effect and chiral magnetic wave using pPb collisions in 2017, which opened a new window in search for anomalous chiral effects in lead-lead (PbPb) collisions. Following the first study, Tu carried out a new measurement to precisely quantify the background effect and set the world's best limit on the presence of chiral magnetic effect in nuclear collisions. At Quark Matter 2018 conference held in Venice, Italy, Tu was invited to give a plenary talk on the experimental status of the searches for anomalous chiral effects. Due to his accomplishment, Tu was awarded a Goldhaber Distinguished Fellowship from Brookhaven National Lab to continue his scientific career there. Postdoc, Zhenyu Chen, continued his studies on the unexpected novel fluid-like behavior of nuclear matter created in small pPb collision, with a new focus on the behavior of heavy mass quarks, such as charms. Fluid-like collectivity of charm quarks was previously observed in PbPb collisions but was not expected in pPb system. With high precision data he coordinated to collect, Chen was able to make the first observation of a nonvanishing collective signal for charm quarks in pPb. This finding requires new theoretical understanding of hot and dense nuclear matter in the limit of very small system size (~ 1 fm). The goal of the group next is to start probing the effect of vorticity in the fluid-like medium formed at trillion degrees in high-energy nuclear collisions.

WEN-HONG LI, I-1902, The University of Texas Southwestern Medical Center. FLUORESCENT PROBES FOR CELLULAR IMAGING.

Numerous mammalian cells contain abundant Zn²⁺ in their secretory granules. During stimulated secretion, Zn²⁺ is coreleased with other cargos into the extracellular medium, and the released Zn²⁺ can function as an important signal to modulate the biochemistry of neighboring cells or distant cells via paracrine or endocrine mechanisms. Despite the biological importance of granular Zn²⁺ activity, it remains challenging to monitor Zn²⁺ levels in the lumen of secretory granules with high specificity and sensitivity. To fill this technological gap, we have developed a class of cell membrane permeable fluorescent zinc granule indicators, ZIGIRs, that displayed more than 30-fold fluorescence enhancement upon Zn²⁺ binding. ZIGIRs are acidophilic, yet their fluorescence is refractory to pH fluctuation down to pH 5 so they are ideally suited for measuring Zn²⁺ in acidic compartments including secretory granules. In pancreatic islet beta cells, ZIGIRs mark Zn²⁺-rich insulin granules with high specificity and reveal dynamic movements of individual insulin granules in living cells by time-lapse imaging. In addition to fluorescence microscopy, ZIGIRs are also compatible with flow cytometry to enable sorting of heterogenous beta cells based on their insulin granule contents. When combined with a fluorescent conjugate of exendin-4 peptide, ZIGIR-2 enabled sorting primary mouse islet cells into highly enriched α -cell, β -cell and δ -cell. Flow cytometry analysis also revealed the hitherto unknown higher Zn²⁺ activity in the glucagon granule than in the somatostatin granule. We expect ZIGIRs to have wide applications for studying the regulation, biogenesis and trafficking of Zn²⁺-rich granules in living cells and for engineering beta cells with high insulin contents for treating diabetes. A manuscript describing this work is under review.

XIAOQIN (ELAINE) LI, F-1662, The University of Texas at Austin. BIO-COMPATIBLE QUANTUM SENSORS.

We previously reported experimental demonstration of a new type of plasmonic sensor consisting of a single metallic nanoparticle and a single semiconductor quantum dot. A quantum two-level system, i.e., the exciton resonance in a single semiconductor quantum dot interferes with a classical system, i.e., the plasmonic resonance in a gold nanoparticle, leading to a Fano resonance mediated by single photon scattering event. This result represents a critical step in realizing hybrid sensors consisting of genuine quantum systems. In this grant year, we continue to work in the fruitful area of hybrid photonic materials and sensors. In this grant year, we have published 1 article in Physical Review B and 1 article in Scientific Report. In addition, we have submitted several papers to high impact journals. One paper has been accepted in Physical Review Letters, and another paper has been accepted by Nature Physics. In the paper published in Physical Review B, by comparing the spectral shift between the exciton resonances measured in linear absorption and photoluminescence experiments, one can use Stokes shift to measure to quantify the degree of disorder. In the Scientific Report article, we explore the loss mechanism of highest

quality single crystalline Ag. By comparing the surface plasmon polariton propagation distance at low and room temperatures, we found that phonon-electron scattering contribute significantly to noble metal loss at room temperature. In the Physical Review Letter article, we discovered a unique quantum index, valley, associated with the defect-bound excitons on a semiconductor monolayer exhibit a lifetime exceeding microseconds. Finally, in the Nature Physics article, we explore the exceptionally large exchange interaction in semiconductor monolayers lead to multiple biexciton resonances.

EREZ LIEBERMAN AIDEN, Q-1866, Baylor College of Medicine. **MAPPING CHROMATIN LOOP DYNAMICS IN DIFFERENTIATING HEMATOPOETIC CELLS.**

Strikingly, we observed the formation of hundreds of long-range loops between large, repressed canyons lying on the same chromosome, as well as evidence for links between DNA methylation canyons lying on different chromosomes. Taken together, our data are consistent with the formation of a unique set of hubs in which large DNA methylation canyons from across the genome tend to co-segregate.

Loops of this extraordinary size have rarely been reported except on the inactive X chromosome (Rao et al., 2014; Darrow et al., 2016), so we next sought to determine whether they were a general feature of primary hematopoietic cells. To this end, we sought to characterize long-range interactions by Hi-C in two HSPC progeny lineages that we could also obtain from human UCB, namely T-cells and erythroid progenitors (EPs). T-cells were isolated using FACS for CD3+ cells, and EPs were generated via directed differentiation (see methods) and then sorted as CD36+ CD71+ CD235a+ cells. For each cell type, we generated nearly ~1B read pairs representing 622M, and 857M contacts respectively (Table S1). We found that these features are present, albeit much weaker, after HSPC differentiation and in other differentiated cell types.

Thus, our surprising findings indicate that DNA methylation works in tandem with histone modifications to influence the 3D architecture of the human genome.

Notably, we have also successfully developed the Hi-Culfite protocol for simultaneous characterization of 3D genome architecture as well as mapping of methylation genome-wide. This promising method has already been adopted by NIH's Encyclopedia of DNA Elements (ENCODE) Consortium, and we have been funded to generate dozens of Hi-Culfite maps in hematopoietic cells and beyond.

PAUL A. LINDAHL, A-1170, Texas A&M University. **CHARACTERIZATION OF LOW-MOLECULAR-MASS METAL COMPLEXES IN MITOCHONDRIA AND BLOOD.**

We published 2 papers this past year with support from the Robert A. Welch foundation. The first study, Moore et al. (2018), characterized the Mrs3D/Mrs4D (DD) yeast strain in which Mrs3/4, the high-affinity iron importers on the mitochondrial inner membrane, were deleted. We used Mössbauer, EPR, and UV-vis spectroscopies, as well as an anaerobic liquid chromatography system interfaced to an online inductively coupled plasma mass spectrometer (LC-ICP-MS). We found that the DD mitochondria shifted from a diseased state to a healthy state with increased levels of iron in the medium, and we developed a chemical model that explains these changes in yeast cells. We also obtained new insights regarding the identity and role of an iron complex with an approximate mass of 580 Da. This species may be used as feedstock for iron-sulfur cluster assembly. The second study, Dziuba et al. 2018, used the same LC-ICP-MS system to detect and investigate low-molecular-mass iron complexes in blood from various mammals. Such iron, referred to as Non-Transferrin-Bound Iron (or NTBI), is pathogenic in iron-overload diseases. NTBI has been considered to be ferric citrate for years. We detected a half-dozen iron species with masses between 400 – 2500 Da; they are present at only nanomolar concentrations.

These species had a unique chromatography profile, distinct from ferric citrate; thus we conclude that these species are not ferric citrate as commonly assumed. We also submitted 3 manuscripts in which the Welch Foundation is acknowledged; one describes a math model of iron trafficking and regulation in yeast cells, one describes a biophysical investigation of the iron content of Escherichia coli, and the third is a review of the mechanistic enzymology of acetyl-coenzyme A synthase/carbon monoxide dehydrogenase. Next year, we will focus on a zinc complex found in E. coli with an apparent mass of 1500 Da using ESI-MS and NMR spectroscopies. Similar Zn complexes are present in yeast.

STEPHAN LINK, C-1664, Rice University. **OBSERVING CHEMISTRY VIA SURFACE PLASMONS.**

Light emission from metallic nanoparticles is typically weak. However, due to the absence of photobleaching, single Au nanoparticles can be easily observed in a microscope. The origin of the emission has recently been debated. It was suggested to be due to electronic Raman scattering. We have argued though that it is caused by the radiative recombination of hot carriers. To prove this mechanism we studied the single particle emission spectra of 80 Au nanorods as a function of excitation wavelength above and below the interband threshold. We were able to establish that photons are emitted following both inter- and intraband pathways. Our theoretical model quantitatively agrees with the experimental results. This model treats the photoluminescence as the radiative recombination that is enhanced by the large photonic density of states (PDOS) created by the plasmon. We showed that the PDOS enhancement and hence the photoluminescence quantum yield depend on the quality factor of the plasmon. Au nanorods fabricated by electron-beam lithography are polycrystalline, have broader resonances and poorer quality factors, and give lower emission. Coating the surface of Au nanorods with Pt islands strongly quenches their emission. Together with single particle absorption and scattering spectra we concluded that hot carriers transfer from Au to Pt. Using femtosecond pump-probe spectroscopy we investigated directly the time-dependent energy relaxation in nanostructures, including the excitation of coherent phonon modes. We found that the phonon modes in nanoparticle clusters couple with each other via the supporting substrate and that their damping is stronger in polycrystalline nanostructures compared to chemically synthesized colloidal samples. Finally, we developed a method capable of acquiring 100 scattering spectra in parallel with a 1 ms integration time in order to follow irreversible chemical reactions. We also wrote a review article on single particle absorption spectroscopy.

JEN LIOU, I-1789, The University of Texas Southwestern Medical Center. NOVEL IMAGING PROBES FOR INVESTIGATING ER-PLASMA MEMBRANE CONTACT SITES.

A). Using imaging probes developed in previous grant years and two super-resolution imaging techniques - photo-activated localization microscopy (PALM) and structural illumination microscopy (SIM), we reveal the size and shape of single ER-PM contacts and show that cortical actin contributes to spatial distribution as well as stability of ER-PM contacts. Our findings were published in an article entitled "Cortical actin contributes to spatial organization of ER-PM junctions" in the 2017 Special Issue on Quantitative Cell Biology of Molecular Biology of the Cell. In addition, we were invited to present this work at a mini-symposium of the 2017 joint ASCB | EMBO meeting in Philadelphia, Pennsylvania.

B). We have developed additional imaging probes named iMAPPERS which enable us to investigate the regulation of store-operated calcium entry at ER-PM contact sites by the interaction between the ER calcium sensor protein STIM1 and the microtubule plus-end binding protein EB1. The findings were published in an article entitled "EB1 binding restricts STIM1 translocation to ER-PM junctions and regulates store-operated calcium entry" in the Journal of Cell Biology. In addition, I was invited to present this work at the 2018 Signaling at Membrane Contact Sites meeting in Doha, Qatar, and at the 2018 FASEB conference on Calcium and Cell Functions: From Mechanisms to Diseases at Lake Tahoe, California.

C). We have characterized two new imaging probes that selectively label ER contacts with late endosomes and lysosomes, respectively. We have applied these two probes to investigate ER contacts with different late endocytic compartments during cholesterol trafficking in mammalian cells. I have been invited to present this work at the 2018 Gordon Research Conference on Lysosomes and Endocytosis in Andover, New Hampshire. A manuscript describing these findings is being prepared.

HUNG-WEN LIU, F-1511, The University of Texas at Austin. MECHANISTIC STUDIES OF NOVEL ENZYMES.

The structure of spectinomycin contains a central dioxane ring that is linked to an actinamine aglycone and the 3-ketosugar actinospectose. Our efforts during this period have focused on studying the cyclization step that leads to formation of the dioxin ring during biosynthesis of spectinomycin. We have successfully expressed and purified the radical SAM enzyme SpeY, which has been proposed to be responsible for the cyclization step. We also chemically synthesized several putative cyclization precursors including (5S)- 4-keto-tetrahydrospectinomycin, (4R)- and (4S)-dihydrospectinomycin. However, none of these were processed when incubated with SpeY. It was later found that the over-reduced (4R)- tetrahydrospectinomycins could be turned over by SpeY. As a result, both (4R,5S)- and (4R,5R)- tetrahydrospectinomycin were prepared by chemical reduction of (4S)-dihydrospectinomycin and tested for their competence as the substrate for SpeY. Our results revealed that both are substrates for SpeY. The product was characterized to be (4S)-dihydrospectinomycin by HPLC co-elution with an authentic standard, high-resolution MS, and NMR. Preliminary data indicated that (4R,5R)-tetrahydrospectinomycin is a better substrate for SpeY. The (4R,5R)-[5-2H]-tetrahydrospectinomycin (> 98% D) was also synthesized. Upon incubation with SpeY, 77% of deuterium was incorporated into 5'-deoxyadenosine, which implies that the reactive 5'-deoxyadenosyl radical generated via the radical SAM machinery in the active site of SpeY abstracts the C5 axial hydrogen during the cyclization. Future efforts will be devoted to the elucidation of the reaction stoichiometry, enzyme kinetics, and cyclization mechanism.

JUN LIU, AU-1714, The University of Texas Health Science Center at Houston. HIGH-RESOLUTION STRUCTURE DETERMINATION OF MOLECULAR MACHINES IN SITU BY CRYO ELECTRON TOMOGRAPHY.

Vibrio species are Gram-negative rod-shaped bacteria that are ubiquitous and often highly motile in aqueous environments. Vibrio swimming motility is driven by a polar flagellum covered with a membranous sheath, but this sheathed flagellum is not well understood at the molecular level because of limited structural information. Here, we use *Vibrio alginolyticus* as a model system to study the sheathed flagellum in intact cells by combining cryo-electron tomography (cryo-ET) and sub-tomogram analysis with a genetic approach. We reveal striking differences between sheathed and unsheathed flagella in *V. alginolyticus* cells, including a novel ring-like structure at the bottom of the hook that is associated with major remodeling of the outer membrane and sheath formation. Using mutants defective in flagellar motor components, we defined a *Vibrio*-specific feature (also known as the T ring) as a distinctive periplasmic structure with 13-fold symmetry. The unique architecture of the T ring provides a static platform to recruit the PomA/B complexes, which are required to generate higher torques for rotation of the sheathed flagellum and fast motility of *Vibrio* cells. Furthermore, the *Vibrio* flagellar motor exhibits an intrinsic length variation between the inner and the outer membrane bound complexes, suggesting that the outer membrane bound complex can shift slightly along the axial rod during flagellar rotation. Together, our detailed analyses of the polar flagella in intact cells provide new insights into unique aspects of the sheathed flagellum and the distinct motility of *Vibrio* species.

QINGHUA LIU, I-1608, The University of Texas Southwestern Medical Center. CHEMOSENSING MECHANISM OF THIAZOLINE ODOR-EVOKED INNATE FEAR.

Innate behaviors are genetically encoded, but their underlying molecular mechanisms are largely unknown. Predator odor 2,4,5-trimethyl-3-thiazoline (TMT) and its potent analog 2-methyl-2-thiazoline (2MT) are believed to activate specific odorant receptors to elicit innate fear/defensive behaviors in naïve mice. Here, we conducted a large-scale recessive genetics screen of ethylnitrosourea (ENU)-mutagenized mice. We found that loss of TRPA1, a pungency/irritancy receptor, diminished TMT/2MT and snake skin-evoked innate fear/defensive responses. Accordingly, *Trpa1*^{-/-} mice failed to effectively activate known fear/stress brain centers upon 2MT exposure, despite their apparent ability to smell and learn to fear 2MT. Moreover, TRPA1 acted as a

chemosensor for 2MT/TMT and TRPA1+ trigeminal ganglion neurons contributed critically to 2MT-evoked freezing. Our results indicate that TRPA1-mediated nociception plays a crucial role in predator odor-evoked innate fear/defensive behaviors. The work establishes the first forward genetics screen to uncover the molecular mechanism of innate fear, a basic emotion and evolutionarily conserved survival mechanism.

WENSHE LIU, A-1715, Texas A&M University. NOVEL CHEMICAL BIOLOGY TOOLS FOR INVESTIGATING THE PROTEIN UBIQUITINATION SYSTEM.

In the previous year, we reported an invented technique that allowed the genetic incorporation of Ne-(4-azidobenzoyl)-d, e-dehydrolysine (AcdK) into ubiquitin for its further conjugation with another ubiquitin component. This work was reported in *Angewandte Chemie*. To improve the incorporation efficiency of AcdK in a bacterial expression system, we optimized our pyrrolysyl-tRNA synthetase mutant (AcdKRS) that was originally evolved for the incorporation of AcdK at an amber mutation in a targeted gene in *E. coli* cells. By randomizing the N-terminal domain of AcdKRS, we constructed a large AcdKRS mutant library. Selection from this library for suppression of an amber mutation in superfolder GFP allowed us to identify several highly efficient clones for AcdK incorporation. This result has been reported in the journal *ChemBioChem* as a cover feature article. In the previous year, we reported a novel discovery that potentially allows functionalization of any protein that has no internal cysteine residues. This is based on the activation of a cysteine genetically installed at a protein C-terminus by 2-nitro-5-thiocyanatobenzoic acid and a followup reaction with an alkyl amine. We have tested this technique in both ubiquitin and most of ubiquitin-like proteins that have been identified in human. They can all be functionalized in their C-termini in this way. We have even synthesized ubiquitin and ubiquitin-like proteins with a propargyl amine C-terminus and used them as activity-based probes for pulling down deubiquitinases in human cells that hydrolyze ubiquitin and ubiquitin-like proteins from their conjugating partners. A manuscript describing this progress is under preparation. Now we are extending the technique to synthesize di- and triubiquitins.

XIN LIU, I-1790, The University of Texas Southwestern Medical Center. STRUCTURAL BASIS AND CHEMICAL MODULATION OF GENE SILENCING BY POLYCOMB REPRESSIVE COMPLEX 2.

In this grant year, we published three peer-reviewed papers that are summarized below. (1) In collaboration with Tom Cech's lab from University of Colorado Boulder and a Pfizer research group, we published an *eLife* paper, where we used comprehensive mutagenesis, RNA-binding EMSA assays and hydrogen deuterium exchange mass spectrometry (HDX-MS) to identify critical residues for RNA interaction in PRC2 core complexes from *Homo sapiens* and *Chaetomium thermophilum* (ct). We found that key RNA-binding residues are mainly dispersed on the different surfaces of Ezh2. This study provided a paradigm for RNA binding by other chromatin complexes without canonical RNA-binding motifs. (2) In a *Molecular Cell* paper, we reported the crystal structures of a 120 kDa heterotetrameric complex consisting of Suz12, Rbbp4, Jarid2, and Aebp2 fragments that is minimally active in nucleosome binding. We found that Suz12 contains two unique structural platforms that define distinct classes of PRC2 holo complexes for chromatin binding. In addition, we showed that nucleosome binding enabled by Jarid2 and Aebp2 is in part accounted for by the structures, which also reveal that disruption of the Jarid2-Suz12 interaction may underlie the disease mechanism of an oncogenic chromosomal translocation of Suz12. (3) In a paper on *Scientific Reports*, we solved crystal structures of both human and ctPRC2 bound to GSK126 and the structurally similar inhibitor GSK343. Our data indicated that while the two organisms feature a disparate degree of inhibitor potency, surprisingly, GSK126 binds in a similar manner in both structures. Structure-guided protein engineering of the drug binding pocket allowed us to introduce humanizing mutations into ctEzh2 to produce a ctPRC2 variant that is more susceptible to GSK126 inhibition. We concluded that a conserved structural platform dictates a unique mode of GSK126 binding, suggesting a mechanism of drug selectivity.

YI LIU, I-1560, The University of Texas Southwestern Medical Center. BIOCHEMICAL ANALYSIS OF AN RNA INTERFERENCE PATHWAY.

Most amino acids are encoded by two to six synonymous codons. Synonymous codons are not used with equal frequencies in all organisms, a phenomenon called codon usage bias. Selection pressure for efficient translation of highly expressed genes was thought to be the major cause of codon usage bias. Even though codon usage bias has been known for decades, its biological functions are not clear and most of the previous studies have been at the level of bioinformatics or in prokaryotic systems. In the past funding period, we studied the role of codon usage in regulating protein folding and gene expression. In the first study, we used a *Drosophila* cell-free translation system to directly compare the velocity of mRNA translation elongation. Our results demonstrate that optimal codons speed up translation elongation while non-optimal codons slow down. In addition, codon usage regulates ribosome movement and stalling on mRNA. Finally, we show that codon usage affects protein structure and function. Together, these results suggest that the effect of codon usage on translation elongation speed is a conserved mechanism from fungi to animals.

In the second study, using *Neurospora* as a model organism, we demonstrated that introduction of rare codons results in premature transcription termination (PTT) within open reading frames and the abolishment of full-length mRNA. PTT is a wide-spread phenomenon in *Neurospora* and there is a strong negative correlation between codon bias and PTT events. Rare codons lead to the formation of putative poly(A) signals and PTT. A similar role for codon usage bias was also observed in mouse.

Together, these results suggest that codon usage biases co-evolve with the transcription termination machinery to suppress premature termination of transcription and thus allow for optimal gene expression.

In addition to these studies, we also carried out a study concerning mechanism of circadian clock.

STEVE W. LOCKLESS, A-1742, Texas A&M University. MEMBRANE PROTEIN REGULATION THROUGH THE LIPID BILAYER.

In addition to the three published papers, we investigated the physical chemical properties of the Kch K⁺ channel and its endogenous role in *E. coli*, which led us to discover the first essential role of bacterial K⁺ channels. We hypothesize that a primary role of K⁺ channels in bacteria is buffering the membrane potential during rapid growth. This is necessary because the enormous flux of electrons through the electron transport chain (ETC) during growth can lead to extreme membrane hyperpolarization. Hyperpolarization potentially alters essential biological processes, such as membrane protein translocation, ETC efficiency, and solute and Lipid II transport, or it can physically disrupt the integrity of the membrane.

This hypothesis is based on several experimental results: 1) Kch is regulated by adenosine nucleotide containing molecules, like NADH, which provides electrons to the ETC and drives rapid proton efflux that can lead ultimately to the extreme hyperpolarization, 2) deletions of K⁺ channels in *E. coli* and *B. subtilis* are lethal unless suppressor mutations arise that make the ETC less efficient, suggesting a conserved role for bacterial K⁺ channels, and 3) the membrane potential of Kch deletion strains are more hyperpolarized compared to parental strains. We are currently preparing a manuscript to describe this essential role for bacterial K⁺ channels.

In the future, we will focus on understanding why extreme hyperpolarization leads to cell death and also on the role of lipids in regulating the Kch channel. Intriguingly, the inexplicable banding pattern we previously observed on motility plates during growth of Kch and some ETC protein deletion strains are also seen in mutations that alter cardiolipin synthesis. This phenotypic link between Kch, the ETC and lipid biosynthesis suggests that the composition of the lipid membrane might be regulating the K⁺ channel and/or ETC proteins. Further work is needed to test this link at the physical level.

JUN LOU, C-1716, Rice University. DEVELOPING ATOMIC LAYER ENABLED TUNABLE AND FLEXIBLE PHOTODEVICES.

We have been continuing making good progress. A few selected projects are highlighted here. We fabricated a vertical GaTe-InSe van der Waals (vdWs) p-n heterojunction by a PDMS-assisted transfer technique without etching. The fabricated p-n heterojunction shows gate-tunable current-rectifying behavior with a rectification factor reaching 1000. In addition, it features fast photodetection under zero bias as well as a high power conversion efficiency (PCE). Under 405 nm laser excitation, the zero-biased photodetector shows a high responsivity of 13.8 mA/W as well as a high external quantum efficiency (EQE) of 4.2%. Long-term stability is also observed and response time of 20 μ s is achieved due to stable and fast carrier transits through the built-in electric field in the depletion region. This fast and efficient charge separation in a vertical 2D p-n junction paves the way for developing 2D photodetectors with zero dark current, high speed and low power consumption. We also developed a synergistic strategy to obtain highly enhanced photoluminescence (PL) of monolayer MoS₂ by simultaneously improving the intensity of the electromagnetic field around MoS₂ and the QY of MoS₂. Self-assembled sub-monolayer Au nanoparticles underneath the monolayer MoS₂ and bis(trifluoromethane)sulfonimide (TFSI) treatment to the MoS₂ surface are used to boost the excitation field and the QY, respectively. An enhancement factor of the PL intensity as high as 280 is achieved. The enhancement mechanisms are analyzed by inspecting the contribution of the PL spectra from A excitons and A trions under different conditions. Our study takes a further step to developing high-performance optoelectronic devices based on monolayer MoS₂. Finally, a novel crystal configuration of sandwiched S-Mo-Se structure (Janus S-MoSe) at the monolayer limit has been synthesized and carefully characterized.

CARL J. LOVELY, Y-1362, The University of Texas at Arlington. TOTAL SYNTHESIS OF SPIROCYCLIC MARINE SPONGE-DERIVED ALKALOIDS

Recently, we discovered an oxidative dearomatization reaction of propargyl guanidines that delivered the complete spirocyclic framework found in the sponge metabolites spirocalcaridine A and B in one chemical operation. We have continued to explore this chemistry on two fronts: (a) Application to the total synthesis of the spirocalcaridines and (b) investigating the scope and mechanism of the transformation. In terms of progress towards the total synthesis we have encountered problems associated with the rearrangement of the spirocyclohexadienone while attempting to isomerize an olefinic functionality. To circumvent this issue, reduction of all the unsaturation has permitted functional group manipulation. Adjustment of the oxidation state of the framework is all that remains to complete the synthesis. In terms of addressing the scope of the chemistry, we have examined propargyl urethanes, and allylic urethanes; both are competent substrates. We have also investigated substrates that lack the alkyne, specifically benzylic ureas and thioureas, and found that they will afford either the benzofused azole (oxazole or thiazole) or the corresponding spiro fused cyclohexadienone. In our oxidative rearrangement chemistry, while this area is more mature, surprises keep arising. Most notably, we have discovered that some 2-azido substituted systems give anomalous rearrangement products, specifically delivering two types of tetrazoles. In one example, this is a case of post rearrangement valence tautomerism of the initially formed azido-azomethine. One additional surprise in this area was an unexpected stereochemical outcome of an oxidative rearrangement which based on established precedent from our studies, occurred from the more nominally sterically hindered face of a polysubstituted tetrahydrobenzimidazole. Studies are currently underway to establish the origin of this selectivity and to develop solutions such that progress towards our targets continues.

VASSILY LUBCHENKO, E-1765, University of Houston. BONDING AND STRUCTURAL DEGENERACY IN INCOMMENSURATE PHASES AND QUASICRYSTALS.

1. We have computer-generated, for the first time, high quality structures for a technologically important family of amorphous inorganic compounds, called the chalcogenides, that consistently exhibit all types of electronic states thought to exist in glassy semiconductors: The bands of delocalized states comprising the mobility bands, the localized states comprising the exponential Urbach tail, the mysterious midgap electronic states, and the polaron-like states deemed to be the dominant charge carrier. We have shown the midgap states are the source of charge carriers, thus obviating existing views.

2. We have unified, for the first time, the microscopic pictures for the structural glass transition in molecular liquids and the jamming transition in particulate systems such as colloids. We have found the two regimes are separated by a spinodal line of instabilities intimately related to the crossover between collisional and activated transport in equilibrated melts. We have disproved a proposed connection between the meanfield Gardner instabilities and the puzzling low temperature anomalies found in glasses.

3. We have conclusively shown that reversible mesoscopic aggregation can take place in equilibrated liquid mixtures, in seeming contradiction with existing paradigms of phase ordering. Thus we have explained the presence of puzzling mesoscopic clusters found in solutions of many proteins and some pharmaceuticals. This interesting and unexpected phenomenon is predicted to occur when solute molecules form sufficiently long-lived transient complexes. We have designed and implemented a novel methodology to detect the presence of such complexes using high resolution mass spectroscopy and Fourier analysis.

4. We have discovered that typical charge density fluctuations in alkali metals result in substantial deformation of the Fermi surface, which upends the traditional view of these materials as simple metals with an isotropic, simply-connected Fermi surface.

ROBERT R. LUCCHESI, A-1020, Texas A&M University. NUCLEAR MOTION PROBED BY MOLECULAR-FRAME PHOTOIONIZATION.

We have studied the multiphoton ionization of NO₂. We considered the effects of electron correlation and of nuclear motion in the five photon ionization leading to dissociation into NO⁺ and O. A comparison of experimental recoil-frame photoelectron angular distributions and their wavelength dependence with theory provided conclusive evidence that there is an initial three-photon absorption to a Rydberg state, followed by a one-photon ionization step, and a subsequent one-photon excitation to a dissociative state of NO₂⁺.

Additionally, we studied the rescattering dynamics of the ethylene molecule when it is subject to intense laser radiation. By a comparison between computed electron-molecular ion scattering differential cross section and measured angle-resolved high-energy electron emission spectra we have shown that it is possible to extract the bond lengths of the molecule to within an uncertainty of 5%. This shows that using rescattering spectroscopy it is possible to obtain time resolved molecular structure with femtosecond time resolution.

LAWRENCE LUM, I-1665, The University of Texas Southwestern Medical Center. FUNCTIONAL INTERROGATION OF EXTRACELLULAR PROTEIN LIPIDATION.

In this final research report we summarize the progress we have made towards a general understanding of:

The influence of lipidation on secreted protein function and b) the role of membrane bound O- acyltransferases (MBOATs) in cell signaling. Using WNT lipidation as a model system, we have delineated cellular innovations required to immobilize a lipid onto a protein in the extracellular milieu that contrast with the molecular devices used to perform a similar feat inside the cell. First, fatty acyl donors are trapped inside the cell and must traverse the lipid bilayer in order to contact a secreted peptide. Thus MBOATs such as PORCN (WNT acyltransferase) likely have transporter-like functions. In the case of WNTs, the requirements of stearoyl co-A desaturase, an intracellular enzyme, for WNT production confirms the intracellular source of fatty acyl donors. Second, using various fatty acyl probes we have demonstrated that the separation of lipidated WNTs from the MBOAT is dependent upon the fatty acyl species - in this case the monounsaturated fatty acid palmitoleate. Despite features within the active site of PORCN that enforce the immobilization of a MUFA, WNTs acylated with a trans FAs fail to extricate from PORCN thus effectively shutting down the production of these aberrantly lipidated WNTs. Finally, we demonstrate that PORCN inhibitors currently in clinical testing disrupt the ability of WNTs to form WNT/PORCN complexes. This action prevents the subsequent transfer of WNT from PORCN to WLS, a chaperone protein for lipidated WNTs, likely by crippling the formation of a ternary complex. In summary, we have provided a mechanistic account of how extracellular protein lipidation is achieved using WNTs as a model system. These observations delineate a research path for interrogating the function of other MBOATs, and for developing additional chemical probes for testing therapeutically relevant hypotheses focused on modulating extracellular protein lipidation.

LLOYD L. LUMATA, AT-1877, The University of Texas at Dallas. TRACKING AMINO ACID METABOLISM IN CANCER IN REAL-TIME HYPERPOLARIZED ¹³C MAGNETIC RESONANCE.

For the 3rd annual report of this Welch grant, we have published 4 peer-reviewed research papers to date on optimized ¹³C dynamic nuclear polarization or hyperpolarized ¹³C NMR: (i) Journal of Physical Chemistry A (DNP with transition metal doping), (ii) Journal of Physical Chemistry B (13C DNP at different magnetic fields), (iii) Journal of Chemical Physics (13C DNP of carbonyl and methyl spins), and (iv) The Journal of Physical Chemistry Letters (invited article on optimization of 13C DNP, article accepted for publication). The first 3 papers herein (JPCA, JPCB, JCP) encompass new physical insights on attaining the highest NMR and MRI signals in DNP, while the high-impact JCP Letters paper is an invited perspective article on 13C DNP optimization. Our DNP research on in vivo application on tumor-bearing mice is still ongoing, and so far our preliminary data indicate that the hyperpolarized [1-¹³C] branched chain amino acids (leucine, isoleucine, and valine), [5-¹³C]glutamine, [1-¹³C]serine, and [1-¹³C]alanine show favorable results as in vivo metabolic NMR/MRI agents, pending more trials for verification. This in vivo cancer research will continue on our recently renewed Welch grant and we anticipate publication of these in vivo results within this year. Overall, the three-year Welch grant support has produced 15 peer-reviewed research publications and counting and supported 3 graduate students (one of them, Welch-supported Peter Niedbalski got his PhD last year and is now a postdoc at Cincinnati Children's Hospital Medical Center). Furthermore, our group has consistently hosted a Welch summer high school scholar for 3 years in a row, the most recent

of which was Sarah Chieng from Austin, TX. In summary, our Welch-supported research has so far been very prolific and we will continue build upon this research momentum with the recently renewed Welch grant.

WEIBO LUO, I-1903, The University of Texas Southwestern Medical Center. REGULATION OF HYPOXIA-INDUCIBLE FACTOR 1 TRANSCRIPTIONAL ACTIVITY BY THE HISTONE MODIFIER.

Major accomplishments

In Year 2, we continued studying HIF-1 α methylation by G9a in GBM cells as planned and made a great progress.

1. We confirmed mono- and di-methylation of endogenous HIF-1 α at lysine (K) 674 by G9a in human U251MG cells.
2. K674 methylation suppressed HIF-1 transcriptional activity and HIF-1 target genes PTGS1, NDNF, SLC6A3, and Linc01132 in U251MG cells.
3. Inhibition of HIF-1 by K674 methylation was due to reduced HIF-1 α transactivation domain function but not increased HIF-1 α protein degradation or impaired binding of HIF-1 to hypoxia response elements.
4. K674 methylation significantly decreased HIF-1-dependent migration of U251MG cells under hypoxia.
5. G9a was downregulated by hypoxia in glioblastoma, which was inversely correlated with PTGS1 expression and survival of patients with glioblastoma. Therefore, our findings uncover a hypoxia-induced negative feedback mechanism that maintains high activity of HIF-1 and cell mobility in human glioblastoma.

Publications

1. Our research supported by the Welch has been published or accepted in three prestigious journals including *Nucleic Acids Res.*, *Cell Mol Life Sci.*, and *Mol Cell Oncol.*
2. We submitted two manuscripts to *Nature Medicine* and *J Biol Chem*, respectively.

Invited talk

1. Epigenetic regulation of HIF-mediated breast cancer progression and metastasis, in the international meeting: *Biology of Cancer: Microenvironment & Metastasis*, Cold Spring Harbor, Oct. 10-14, 2017.
2. Epigenetic regulation of hypoxia response in human cancers, at the Eugene McDermott Center for Human Growth and Development, Dallas, Apr. 20, 2018.

Poster presentation

Bao L, Chen Y, Lai HT, Wu SY, Wang JE, Hatanpaa KJ, Raisanen JM, Fontenot M, Lega B, Chiang CM, Semenza GL, Wang Y, Luo W. Inhibition of hypoxia-inducible factor 1 (HIF-1) transcriptional activity and cell mobility by G9a/GLP-mediated methylation of HIF-1 α . AACR annual meeting 2018, Chicago, Apr. 14-18, 2018.

XUELIAN LUO, I-1932, The University of Texas Southwestern Medical Center. CHEMICAL INHIBITION OF THE HIPPO TEAD-YAP TRANSCRIPTION FACTORS FOR CANCER THERAPY.

The Hippo pathway plays key roles in organ size control, tissue regeneration, and tumor suppression by restricting cell proliferation and growth, and promoting apoptosis. Dysregulation of this pathway has been linked to tumorigenesis. TEA domain (TEAD) transcription factors bind to the co-activators YAP and TAZ, and regulate the transcriptional output of the Hippo pathway, playing critical roles in organ size control and tumorigenesis. However, it remains difficult to target TEAD or YAP/TAZ directly with small molecules for cancer drug discovery. We previously reported that TEADs possess intrinsic “enzyme-like” activities, and undergo autopalmitylation. Palmitate binds to a deep hydrophobic pocket in TEADs, and is required for its stability and transcriptional activities of TEAD-YAP complex. Here we report MGH-CP1 as a potent and selective small molecule inhibitor of TEAD autopalmitylation. In crystal structures, MGH-CP1 binds to the conserved lipid-binding pocket in TEAD2, and displaces palmitate binding. Interestingly, MGH-CP1 allosterically inhibits TEAD-YAP transcriptional activator complex, while maintains TEAD stability and TEAD-Vgll4 repressor complex in cells, thus blocking YAP-dependent transcriptional output. In a large-scale cancer cell lines growth profiling, MGH-CP1 sensitivity correlates significantly with YAP-dependency when intersecting with Cancer Dependence Map analysis. Furthermore, MGH-CP1 significantly inhibits YAP-dependent liver overgrowth in *Lats1/2* liver-specific knockout mouse model and tumor growth in human hepatocellular carcinoma and uveal melanoma xenograft tumor models *in vivo*. Our work suggests that pharmacological inhibition of TEAD is a promising therapeutic approach for the treatment of cancers with deregulated Hippo signaling.

NATHANIEL A. LYND, F-1904, The University of Texas at Austin. SYNTHESIS AND SELF-ASSEMBLY OF COOPERATIVELY CRYSTALLINE BLOCK COPOLYMERS.

In the second year of Welch Foundation support, our laboratory has published eight articles, and attended the 255th ACS Meeting in New Orleans, and will attend the upcoming 256th ACS Meeting in Boston, MA to communicate our results. We have made significant progress on the synthesis of polyether materials using our new mono(μ -oxo)-di(alkyl aluminum) (MOD) initiators and new N/Al adduct catalysts and also gained a deeper understanding of the classical Vandenberg catalyst on which they are based.

We have used our synthetic expertise in polymeric materials to investigate the relationship between polymer structure and ionic conductivity needed for energy storage, and also assisted the Keitz lab in the creation of a new “living” polymerization system where living cells are used as the polymerization catalyst. Importantly, we have published our first paper on cryopreservative polymers that makes use of synthetic techniques developed in our lab, and also unique assays for evaluating the interactions between polymers and ice.

Welch Foundation support has been instrumental to our research in fundamental chemistry of epoxide polymerization and the materials that result. We are excited to begin our third year of Welch support, and are excited about the discoveries that lie ahead. In our next year, understanding the unique reactivity of the N/Al catalysts system and its full impact on materials synthesis will provide important developments in the area of polymerization catalysis, and also provide fundamental insights into group-13 based catalysis and structure.

JIANPENG MA, Q-1512, Baylor College of Medicine. EXPLORING THE CHEMICAL FORCES STABILIZING HUMAN POLYCOMB REPRESSIVE COMPLEX 2.

Epigenetic regulations are essential for the government and maintenance of homeostasis. PRC2 is a master epigenetic regulator that controls cell growth, differentiation and stem cell pluripotency. Dysregulation of PRC2 is linked to the initiation and invasiveness of many types of cancer. Consequently, PRC2 complex has been an attractive target for medical intervention of tumors. Long non-coding RNAs (LncRNAs) have important implications in PRC2 regulation. However, until now, a high-resolution structure of human PRC2 with lncRNA is still lacking, which severely hinders the development in this direction. In the past year, we have made major progress in structural determination of PRC2 with its interacting lncRNA by high-resolution single particle cryo-EM reconstruction. We have successfully assembled PRC2-lncRNA complex and purified it to high purity. We have also obtained the optimal freezing conditions and collected a large set of cryo-EM data of the complex. Three dimensional reconstruction of the PRC2-lncRNA complex structure is currently underway.

ALLAN H. MACDONALD, F-1473, The University of Texas at Austin. SPINTRONICS IN TWO-DIMENSIONAL MATERIALS.

My Welch grant supports theoretical research that is directed toward advancing understanding of the electronic properties of graphene sheets and other two-dimensional systems, including single and few layer transition metal dichalcogenides systems and the surface states of topological insulators. One important element of the physical properties of two-dimensional materials is the appearance of moiré patterns when two-dimensional materials with different orientations or with different lattice constants are overlaid. This research includes work with a fundamental physics emphasis and work that also has an eye toward applications. In the past year a major discovery has been made by a research group led by Pablo Jarillo-Harerro at MIT based on earlier Welch supported theoretical research in my group. We have previously identified 'magic angle bilayer graphene' (MABG) as an attractive host for strong correlation physics. It has now been demonstrated that MABG exhibits many of the same phenomena as strongly correlated cuprate superconductors. Much of the work currently in progress has been redirected by this discovery. All this new research is intimately connected to the study of topological matter, including topological insulators, and topological superconductors and the surface states that are associated with the topological properties of these materials which may play a role in future quantum technologies.

FREDERICK M. MACDONNELL, Y-1933, The University of Texas at Arlington. PHOTOTHERMOCHEMICAL LIQUID HYDROCARBON SYNTHESIS FROM WATER AND CARBON DIOXIDE.

We were investigating a photothermochemical process for the conversion of CO₂ and steam into higher hydrocarbons and O₂, so-called 'reverse combustion'. The basic premise of this proposal was the subject of a PNAS paper (Proc Natl Acad Sci USA, 2016, 113:2579–2584) published by myself and co-authors. Unfortunately, we have since retracted this paper (Proc Natl Acad Sci USA, 2018, 115(30) E557) on the basis that the observed higher carbon number hydrocarbons were actually artifacts that were generated from residual graphitic carbon in the commercial P25 TiO₂ we purchased. This TiO₂ contains 0.0120% carbon by mass (or 120 ppm carbon) and we can now show that the combination of UV irradiation and temperatures of 200 C are able to mobilize this carbon to produce the products observed. While we had conducted 13-carbon isotopic labeling experiments at 30% labeling of the CO₂, when these experiments were repeated with 100 % 13-carbon, the label was not observed in the product. The retraction is included in the publications attached.

Given this latitude, I redirected my Welch funding to an long standing project in my lab studying the mechanism of action by which redox-active ruthenium polypyridyl complexes selectively induce apoptosis in malignant cells over non-malignant cells. Two Ru complexes, in particular, show a ten-fold increase selectivity for targeting malignant cells and show anti-tumor activity in mouse tumor models (83% regression). My Welch support is now being used to determine the chemical mechanism of action for DNA damage and demonstrating that these mechanisms, established in vitro, are active and responsible for induction of apoptosis in malignant cells. We have made substantial progress on this project.

Publications include two EJIC papers that acknowledge a previous Welch grant (Y-1301) to FMM.

CORINA MAEDER, W-1905, Trinity University. MECHANISM OF A SMALL PROTEIN AT THE HEART OF SPLICEOSOME ACTIVATION.

To address the hypothesis that Dib1 regulates spliceosome assembly through its interactions with U5 snRNA, two aims were proposed to characterize U5 snRNA-Dib1 interactions biochemically and genetically and then perform single molecule to determine kinetics information about the departure of Dib1.

Over the past year, we published our work (Schreib et al, 2018) showing that Dib1 mutants stalled in vitro splicing and spliceosome assembly in a manner consistent with their growth phenotype. We also demonstrated that exogenous Dib1 could rescue splicing defects, which is quite significant as only a handful of other splicing proteins are able to function this way. This allowed us to speculate that Dib1 is a linchpin in assembly.

We also made significant progress towards addressing our hypothesis related to U5 interactions. In addition to analyzing U5-Dib1 interactions, last year, we described the need for a snRNP composition assay. We have optimized that assay and are exploring the snRNP composition of U5-Dib1 mutants. In a

new collaboration with a computational biophysicist, we performed MD simulations of the B complex and identified a novel set of interactions between U5 snRNA and Dib1, which we are constructing biochemically. Inclusion of computational methods has proved powerful, as the data we extracted from MD simulations aligns with the biological phenotypes we observe for Dib1 mutants (manuscript in prep). For Aim 2, although our single molecule system is based on prior work, Dib1 has posed significant challenges. The Dib1 protein is especially sticky and results in non-specific binding to the slide, leading to high background. We are improving this background problem by modifying slide preparation procedures. In spite of these challenges, our preliminary data suggest that we are achieving splicing of ~13% of the molecules on the slide. Therefore, we expect to assess effects of U5 mutants on Dib1's interaction with the spliceosome shortly.

DMITRII E. MAKAROV, F-1514, The University of Texas at Austin. THEORY AND SIMULATIONS OF SINGLE-MOLECULE DYNAMICS.

1. A new formula was derived, which allows one to estimate the coordinate dependence of the diffusivity directly from single-molecule trajectories.
2. A new inequality was derived, allowing one to test whether or not a single-molecule signal $x(t)$ is a Markov process without memory. This "Markovianity" test works even when the time resolution of the experiment is lower than the characteristic memory time. It is expected that this test will help settling the much debated question of applicability of one-dimensional diffusion models to single-molecule force spectroscopy data.
3. Exact rate theory was reformulated in terms of experimental observables accessible via single-molecule force spectroscopy measurements. The coarse grained transition path velocity introduced in this work (i) is measurable despite limited experimental time resolution, (ii) allows one to define an average shape of transition path that is internally consistent with the observed transition rate, regardless of the underlying dynamics of the experimental signal, and (iii) leads to an intuitively appealing formula for the exact transition rate that has a transition-state-theory-like appearance.
4. In collaboration with the group of Prof. Benjamin Schuler (University of Zurich), experimentally measured distributions of transition path times for the binding of two proteins were analyzed using the theory previously developed by the Makarov group, leading to the conclusion that the binding process involves a short-lived encounter complex.
5. Memory effects on the distribution of transition path times were studied, and new analytical theory was developed that accounts for such effects.
6. The effect of confinement on the dynamics of intrinsically disordered proteins was studied using molecular simulations, leading to new insights into the physical origins of internal friction.

DAVID J. MANGELSDORF, I-1275, The University of Texas Southwestern Medical Center. LIGAND BINDING PROPERTIES OF NEMATODE ORPHAN NUCLEAR RECEPTORS.

For Project 1 we continue to investigate the pharmacologic potential of targeting the nuclear receptor DAF-12 in *Strongyloides stercoralis*, a human nematode parasite. We previously identified the *S. stercoralis* DAF-12 ligand as delta7-dafachronic acid, a ligand that is also found in the free-living nematode, *C. elegans*. This finding brings up the key question of how the parasite acquires the ligand, since parasites lack the analogous enzyme found in *C. elegans* that makes the ligand. We are now addressing this question using both loss and gain of function approaches. For the loss of function approach, we developed a CRISPR system in the parasite (only the second lab to do so) and are now attempting to knockout the 26 orphan cytochrome P450s found in *S. stercoralis*, one or more of which may be the candidate biosynthetic enzyme. For the gain of function approach, we are expressing each of the 26 parasite enzymes in *C. elegans* to try and rescue worms that lack the *C. elegans* enzyme. For Project 2 we made the unexpected discovery that FGF21 is a potent dipsogenic hormone that regulates thirst. We showed that liver-derived FGF21 is required to stimulate water drinking in response to metabolic stresses, such as alcohol intake and ketogenic diets, which can cause dehydration. The effect of FGF21 on water balance is mediated by a hypothalamic circuit that requires beta-adrenergic signaling and, surprisingly, is independent of known thirst circuits. In addition to its beneficial pharmacologic effects on body weight, insulin sensitivity, and lipid levels, endogenous FGF21 protects mice against steatosis and liver injury caused by alcohol or ketogenic diet. Since hydration can affect thermogenesis, body weight, and other metabolic parameters, we are investigating whether some of these salutary actions may be secondary to FGF21's effects on water balance. Efforts in the lab are now focused on identifying this new neuronal circuit.

ARUMUGAM MANTHIRAM, F-1254, The University of Texas at Austin. SYNTHESIS AND PROPERTIES OF TRANSITION METAL OXIDES WITH UNUSUAL VALENCE STATES.

1. The substitution of M^{3+} for Co in swedenborgite $YBaCo_{4-x}M_xO_{7+d}$ enhances the structural stability at the operating temperatures of solid oxide fuel cells (SOFCs) in the order $Ga^{3+} \gg Al^{3+} > Fe^{3+}$. While common perovskite oxide cathodes undergo severe and irreversible degradation in catalytic activity for the oxygen reduction reaction on exposure to air containing CO_2 , such a degradation is drastically reduced with $YBaCo_{4-x}M_xO_{7+d}$ cathodes, which is attributed to the reduced number of oxygen vacancies in the swedenborgite oxides.
2. The exsolved Co-Fe nanoparticles on the surface of perovskite $La_{0.3}Sr_{0.7}Cr_{0.3}Fe_{0.6}Co_{0.1}O_{3-d}$ anodes under the operating reducing condition in SOFCs are self-regenerable through a redox process at 700 – 800 °C; the self-regeneration mechanism is strongly dependent on the redox-reaction temperature. The driving force for the nanoparticle formation is the lowering of metallic surface energy and a strong interfacial interaction between the metal nanoparticles and the metal oxide. The consistent nanoparticle size distribution and high areal particle density before and after the redox process provide unique capability to recover and maintain high, sustainable catalytic activity for fuel oxidation reactions in SOFCs.

3. In a membraneless fuel cell with a catalyst-selective strategy, the use of isopropanol as a fuel eliminates the common carbonate formation problem in KOH since acetone rather than CO₂ is the oxidation product of the fuel; spinel MnNiCoO₄ oxide nanoparticles coupled to multi-wall carbon nanotube surface offers high selectivity for the oxygen reduction reaction.

4. The electrochemical reversibility in lithium-ion cells as well as the stability on exposure to ambient air of the layered LiNi_{1-x}M_xO₂ oxide cathodes with a Ni content of as high as (1-x) = 0.92 has been remarkably improved with a substitution of 2% Al due to enhanced structural robustness and reduced electron delocalization.

EDWARD M. MARCOTTE, F-1515, The University of Texas at Austin. A MASS-SPECTROMETRIC-BASED MAP OF CORE EUKARYOTIC PROTEIN COMPLEXES.

This project uses proteome-scale mass spectrometry to define physical complexes of proteins in organisms spanning the eukaryotic tree of life, helping reveal functions for the many evolutionarily conserved but uncharacterized proteins. The resulting map will serve as a landmark reference of the basic physical wiring diagram of a eukaryotic cell. We made good progress, building on ~6,400 shotgun mass spectrometry proteomics datasets we previously collected on native biochemical fractions from animal cells and tissues (Nature 2015). We've now completed ~2,000 mass spectrometry experiments on diverse plants—by far, the largest plant proteomics experiment ever conducted—to build the first systematic map of plant protein complexes, based on ~50 million protein abundance measurements. We studied important agricultural plants (rice, wheat, tomato, broccoli, soy, coconuts, quinoa, hemp, & algae), found new proteins e.g. in photosynthesis, redox, and gene expression, and found striking parallels and differences between plant and animal protein complexes (to submit in 2018). We integrated our human data with those from the Gygi (Harvard) and Mann (Munich) groups to estimate major protein complexes in human cells (Mol Sys Biol 2017), revealing new proteins in processes linked to birth defects (J Cell Sci 2017; eLife submitted). In all, these data span ~20,000 mass spec experiments, including ~3,000 we performed on ciliates, diatoms, pathogens, and even bacteria (Nature Microbiol 2017). We're now integrating these data on UT supercomputers. We extended our approach to membrane protein complexes by incorporating chemical cross-linking, identified direct protein contacts in our data (PLoS Comp Biol 2017), and found low-res 3D structures of complexes from electron micrographs of mixtures, an approach we named “shotgun electron microscopy” (Cell Reports 2018). We also showed proof-of-concept of a new technology to sequence individual peptide molecules (Nature Biotech, accepted).

CALEB D. MARTIN, AA-1846, Baylor University. HEAVY ELEMENT-BORON SYSTEMS: FROM UNUSUAL BONDING TO NEW SYNTHETIC TOOLS.

This past year we have made some unusual boron complexes through a variety of synthetic pathways. Efforts to construct unusual frameworks have centered on the chemistry of the boron-containing analogue of fluorene, borafluorene. Although this compound was reported in 1963, its reactivity has not been explored. We have found that this species is very reactive and capable of inserting molecules and fragments into the B-C bond. These efforts have resulted in two publications in print (Chemical Communications in a special issue entitled "ChemComm Emerging Investigators 2018" and Organometallics) and an additional manuscript submitted (submitted to Organometallics). We have also had some collaborative work with the Xu group on iron azide catalysis that generated a publication (ACS Catalysis).

With respect to boryl ligands, we have made progress on the preparation of new ligand sets and been able to reproduce the literature methods. Efforts exploring their coordination chemistry are underway.

STEPHEN F. MARTIN, F-0652, The University of Texas at Austin. SYNTHESIS OF BIOLOGICALLY RELEVANT MOLECULES.

A number of important advances in synthesis and chemical biology have been made. We developed new platforms to prepare collections of novel organic molecules for screening against biological targets. We continued to use modulators of sigma2R/TMEM97 in animal models of several neurodegenerative conditions and neurological disorders. We discovered one compound that markedly enhances learning and memory performance and improves neuron and oligodendrocyte survival after traumatic brain injury in two mouse models. A study of the effects of modulators in the 5xFAD model of Alzheimer's disease was initiated. We identified a sigma2R/TMEM97 modulator that protects retinal ganglion cells and photoreceptors in animal models of retinal disease. We identified several sigma2R/TMEM97 modulators that increase survival of neurons in two cellular models of Huntington's disease.

In other areas, we made progress toward the syntheses of alstoscholarisine E, a novel indole alkaloid that promotes neural stem cell proliferation, and we initiated work toward the syntheses of the nonopioid analgesic agent pierisaketolide A and exotine A.

In optogenetic studies to map neuronal circuits in mice, we developed a novel molecule that may be used to cage GABA and a fluorquinolone antibiotic, and we are developing applications of this new caging technique. Significant advantages of this new cage are its water solubility and its ability to be removed quickly with visible light. Proof-of-principle studies involving use of caged erythromycin and anhydrotetracycline are ongoing as a prelude to in vivo studies.

We completed studies of how changes in structures of small molecules that bind to the Src SH2 domain and hepatitis C viral protease affect energetics in their respective bimolecular associations, and we completed additional experiments of inhibitors of the methionyl-tRNA synthetase of *T. brucei*, the parasite that causes African sleeping sickness.

ELISABETH D. MARTINEZ, I-1878, The University of Texas Southwestern Medical Center. **SMALL MOLECULE INHIBITORS SELECTIVELY TARGETING MALARIA EPIGENETIC ENZYMES.**

In the third year of support, we have continued to measure the potency and efficacy of new epigenetic small molecule inhibitors against drug-sensitive and drug-resistant parasite strains. We have identified potent analogs and have begun characterization of their specificity and their overall effects on the life cycle of the parasite as well as on the malaria transcriptome. We have also defined how our top molecules affect histone post-translational modifications in the parasite, by mass spectrometry analysis. This has shown on-target activity. In summary, we have found: 1) that Jumonji inhibitors affect parasite viability long term even after only a transient exposure to the drugs; 2) that the late stage parasites are most sensitive to Jumonji inhibitors; 3) that the inhibitors affect a subset of genes involved in invasion of red blood cells and in gametocyte development. Additionally, we have continued genetic efforts to understand the role of the three Jumonji enzymes encoded by the parasite in order to elucidate their function and selectively target their activities using the epigenetic antimalarial compounds we have developed and are characterizing. Meanwhile, our chemistry efforts also continue with new synthesis of Jumonji inhibitor analogs and testing for potency, efficacy and selectivity of these newly synthesized small molecules. Most importantly, we have written our first manuscript describing all this Welch-funded malaria research and we will be submitting it for publication in the coming weeks.

ANDREAS MATOUSCHEK, F-1817, The University of Texas at Austin. **STRUCTURE AND FUNCTION OF A NANO-SCALE BIOLOGICAL MACHINE.**

Over the last year, we have made progress in four areas related to the project:

1) Inducible degradation of a physiological protein in mammalian culture cells.

We have sought to improve the efficiency of proteasome adaptors by designing a series of adaptors targeting a the physiological protein Shp2. Constructs expressing the adaptors were then transfected into different cells lines to monitor Shp2 depletion. Unfortunately, varying the geometry of the adaptors has so far not led to more efficient depletion. We are now designing adaptors with different interaction modules and developing assays for different target proteins.

2) We have made substantial progress setting up the experiments to define the geometric restrictions on proteasome targeting by designing and purifying some 35 out of the roughly 45 systematically modulated proteasome substrates to be tested. We expect to have the complete set of constructs ready before the end of this calendar year and analyzed before the end of the budget year.

3) We developed two completely independent experimental approaches to investigate the geometry of proteasome-substrate interaction.

a- in collaboration with Jim Reilly, Chemistry, Indiana University, we have developed a covalent cross linking - mass spectrometry approach to define the binding sites of the substrate's ubiquitin chain and initiation region on the proteasome. The information obtained from these experiments will be complementary to the information obtained in experiments described above under point 2. The experiments, funded by the Welch foundation, have led to an NIH grant application.

b- in collaboration with David Taylor, Molecular Biosciences, UT Austin, we have setup experiments to image the proteasome substrate-interaction directly using cryo electron microscopy. Quite surprisingly, we have already been able to obtain images that seem to reveal the position of substrate in the complex, which had not been describe previously.

JEREMY A. MAY, E-1744, University of Houston. **THE TOTAL SYNTHESIS OF BIOACTIVE NATURAL PRODUCTS VIA NOVEL METHODS AND STRATEGIES.**

Objective 1:

Diol-catalyzed enantioselective conjugate addition of organoboron nucleophiles now includes cyclopropyl ketones for homoconjugate addition reactions. We have followed up an earlier report of the use of Bu₄NHSO₄ as a mild and inexpensive catalyst for this transformation with new results that iPrGaCl₃ catalyzes the formation of all-carbon quaternary centers for this reaction, which opens the door for enantioselective catalysis (Org. Lett. 2017). Also, preliminary enantioselectivity has been seen using a new BINOL-based organocatalyst. Very recently, we found that cooperative Lewis and Brønsted acids can perform a related addition to aziridine and azetidione electrophiles. Preliminary reaction development with conjugate addition to vinylogous esters has begun. A historical account of all the work we have contributed in this area has appeared (Synlett 2018), and our expertise has resulted in our being invited to review this area in an upcoming special organocatalysis issue of Molecules. Work toward the synthesis of mucronatins and similar natural product structures continues apace.

Objective 2:

A novel ligand for dirhodium(II) complexes with a BINOL backbone has been synthesized and used to make a highly functional enantioselective catalyst for carbene-based transformations. It's use for the hydrazone-initiated cascades has provided products in ~90% yield and 99:1 er (ACS Catal. 2017). A nitrene-initiated carbene cascade has also been developed that uses a reactive nitrogen species to initiate a cascade reaction that terminates in C-C bond formation via C-H bond insertion. In this cascade, triplet carbenes appear to be active rather than singlet carbenes (Chem. Sci 2017). To better facilitate the synthesis of substrates for this cascade, we have synthesized novel TpRuCl-based catalysts to perform propargylic substitution (Organomet. 2017). Our synthesis of brazilide A also continues.

JENNIFER A. MAYNARD, F-1767, The University of Texas at Austin. CONTROL OF PROTEIN FOLDING QUALITY: PORTABLE SEQUENCE DETERMINANTS OF ANTIBODY STABILITY.

During this period of Welch support, we further developed strategies for high throughput analyses to characterize protein stability and solubility. With Welch supporting one graduate student, this effort has resulted in five published Welch-funded manuscripts in the past year.

Two key papers were published supporting prior Welch efforts. Laber et al showed that changing a protein sequence to include additional charged, solvent-exposed residues decreased protein self- association and aggregation potential at very high protein concentrations (up to 200 mg/ml). Entzminger et al demonstrated our ability to apply knowledge of protein sequence-structure relationships to design an antibody-antigen interaction totally de novo. Starting with a pre-selected protein epitope, antibody binding loops were computationally designed to interact with this epitope and then demonstrated to do so experimentally.

New efforts during the past year included development of a mammalian cell system to display variants of an antibody to select for those with desirable characteristics using flow cytometry (Nguyen et al). In unpublished work, this system has been applied to analyze a protein structurally related to antibodies, the T cell receptor (TCR), and revealed the effects of glycosylation on TCR solubility and stability.

Efforts during the next year will continue to explore the connection between protein sequence, folding and stability for immunoglobulin proteins. Specifically, during the last year, we identified a number of TCR variants which bind the same ligand with similar affinities but only some variants result in cellular activation. Using these TCR variants, we aim to determine the physical factors that discriminate between simple binding and cellular activation.

JULIAN MEEKS, I-1934, The University of Texas Southwestern Medical Center. IDENTIFYING NEW MAMMALIAN BILE ACID RECEPTORS.

We have made strong progress towards the first two proposed Specific Aims in the initial award year. We have utilized live volumetric Ca²⁺ imaging to analyze the bile acid sensitivity and selectivity of more than 10,000 individual neurons in the mouse vomeronasal organ (VNO). We focused our initial efforts on four prominent bile acids: cholic acid (CA), deoxycholic acid (DCA), chenodeoxycholic acid (CDCA), and lithocholic acid (LCA). These experiments produced data indicating the presence of rare populations of neurons that are sensitive to each of these molecules at submicromolar concentrations. We also discovered a population of sensory neurons that are broadly responsive to bile acids and structurally related polar glucocorticoids. These experiments provide a blueprint for further exploration of mouse vomeronasal sensory neuron tuning to bile acids.

We are happy to report that our proposal to use single cell RNA sequencing (scRNAseq) to discover new candidate bile acid receptors has been successful. Though the results are still preliminary, we have established a pipeline using live epifluorescent Ca²⁺ imaging to functionally identify bile acid sensitive and selective neurons, then capture and prepare them for scRNAseq. We identified and processed ~20 bile acid sensitive cells, including CA and DCA "specialists" responding only to 1 uM CA or 1 uM DCA. We also processed ~20 neurons that responded to both 1 uM CA and 1 uM DCA, possibly members of the broadly tuned bile acid- and glucocorticoid-sensitive population. scRNAseq of these neurons, along with comparable numbers of bile acid unresponsive cells, revealed enrichment of 3 vomeronasal receptors: one in CA-selective cells, one in DCA-selective cells, and a third in the broadly-responsive cells. We are now primed and ready to make extensive inroads into bile acid biology as we validate these preliminary results and explore their biological significance.

GABRIELE MELONI, AT-1935, The University of Texas at Dallas. TRANSITION METAL SELECTIVITY AND TRANSLOCATION IN TRANSMEMBRANE ION PUMPS.

Our research addresses the characterization of the principles controlling metal selectivity and transport in several metal transporter families, with focus on two classes of primary active pumps (Cu⁺ and Zn²⁺ ATPases). We have applied a multidisciplinary structural and biochemical strategy on purified prokaryotic Zn pumps to reveal the molecular determinants underlying metal substrate selectivity. We determined the substrate coordination of the transmembrane metal binding site (responsible for substrate selection) in two Zn²⁺/Cd²⁺/Pb²⁺/Hg²⁺ ATPases and revealed the coordination chemistry and structural principles which define their promiscuous selectivity. Biochemical characterization of substrate- dependent ATPase activity coupled to X-ray absorption spectroscopy revealed the existence of a highly- plastic transmembrane high-affinity site that confers selection for defined metals (Zn²⁺/Cd²⁺/Pb²⁺/Hg²⁺) via different coordination geometries and ligand distances, but relying on common bioinorganic properties (to be submitted).

We have also characterized the Cu⁺ binding properties in the purified human copper ATPase ATP7B (collaboration with Dr. Gourdon, Denmark) and compared it to purified bacterial and archaeal copper pumps. The work revealed a uniform principle of metal-handling in Cu⁺ pumps, with one metal associating to each heavy metal binding domain, and a transmembrane domain harboring a single ion binding site, supporting a stoichiometry of one Cu⁺ ion transported per ATP (submitted).

These results are revealing how the strict interplay between the nature of the coordinating ligands, the geometry of metal binding in the transmembrane helices, and the coordination chemistry determine the mechanism by which substrate selection and translocation occurs in P-type ATPase metal pumps. These studies are allowing comparative selectivity, reactivity and mechanistic studies with other metal binding proteins and metal transporter families under our investigation.

OGNJEŠ MILJANIĆ, E-1768, University of Houston. **ROBUST POROSITY IN MOLECULAR CRYSTALS.**

During the past project year, the proposed goals of this project have been advanced along two main directions.

In the first, a range of sixteen new potential precursors to PMCs have been prepared using a combination of Pd- and Cu-mediated coupling reactions and careful manipulations of protecting groups on nitrogen atoms. Upon synthesis, these molecules have been exhaustively characterized, most significantly through X-ray crystallography. This analysis revealed four new porous structures and allowed us to identify structural elements needed for the creation of porosity: trigonal geometry, hydrogen bonding and aromatic pi-pi stacking. The identified porous structures were further characterized by gas sorption and the most porous one was found to have surface area in excess of 1800 m²/g. In addition, precursors to potentially catalytic PMCs have been prepared, using bipyridine-based linkers which will be employed as the anchoring sites for future incorporation of catalytically active metals. Preliminary investigations of proton conductivity have been performed as well on the tetrazole-based PMCs which have infinite one-dimensional chains of hydrogen bonds.

The second research direction focused on the preparation of intrinsically porous molecular crystals based on the cyclotetrazobenzoin skeleton identified previously in our group. We have found that the acetylated derivative of this molecule has a significantly higher surface area than the nonesterified versions. In addition, we have shown that the reduced cyclotribenzoin hexaol self-assembles into hexamers in the solid state, with cavities capable of enclosing a crystallographically ordered water pentamer. Current investigations are aimed at using the central cavity of cyclotetrazobenzoins as a host for molecularly thin guests, such as nitriles and acetylenes.

DELIA J. MILLIRON, F-1848, The University of Texas at Austin. **PLASMONIC TRANSPARENT CONDUCTING OXIDE NANOCRYSTALS: DOPANT CHEMISTRY AND HETEROGENEITY.**

Last year, we investigated influence of surface depletion in IR LSPR. It was discovered that previously neglected semiconductor band structure modifications induced by surface states or applied electrochemical potential strongly affect LSPR modulation [8]. Based on experimental and simulated spectra, surface defect states create a surface depletion layer that alters LSPR properties in electrochemical charge injection and extraction. Surface depletion determined the LSPR frequency modulation extent in ITO nanocrystals in both solution dispersed NC [3] and NC films [8].

Enhanced electronic transport in NC films was achieved by extending our understanding of surface depletion. Surface hydroxyls, detrimental to charge transport, were alleviated by atomic layer deposition

[1] and sol-gel solution infilling [4] to cap bare NC arrays with metal oxides. Synthetic manipulation of dopant selection and distribution further improved conductivity. Incorporating Ce as a dopant allowed high carrier mobility, due to low ionized impurity scattering [4]. Controlled radial dopant distribution of doped shell/undoped core ITO NCs allowed narrow surface depletion width, resulting in higher conductivity and lower contact resistance [1].

Assembly of ITO NC gels, an emergent strategy for multiscale volumetric architectures, was achieved based on physical NC interactions [9]. Long-range electrostatic repulsions between ligand stripped ITO NCs were balanced by short-range attraction from introduction of PEG as a depletant. Intrinsic LSPR was successfully retained while the gel network was formed. In NC film architectures, highly porous, a flexible electrochromic film with rapid electrochromic switching performance was fabricated using WOX nanorods [7]. We observed porous CeO₂ NC films demonstrate significant proton conductivity at elevated temperature due to dissociative adsorption of water at surface oxygen vacancies [5].

SAIKAT MUKHOPADHYAY, I-1906, The University of Texas Southwestern Medical Center. **BIOCHEMICAL CHARACTERIZATION OF FACTORS REGULATING SUBCELLULAR TRAFFICKING AND FUNCTION OF MEMBRANE ADENYLYL/GUANYLYL CYCLASES.**

In aim 1, we are mapping interactions between Ont-1/2 and cyclase domains. Using tandem affinity purification and mass spectrometry with Taplin facility, Harvard University, we are now testing ADCY1/4/8 pull downs, in addition to other ADCYs already performed. We are also planning to perform AC cyclase domain chimera binding experiments with recombinant Ont-1/2.

In aim 2, we are determining if Ont-1/2 affect membrane AC/GC transit through the secretory pathway. We have now generated CRISPR knockouts of Ont-1/2 in stable cell lines expressing tagged ciliary ADCY2, 3, 5, 6, 8 and 9, and working on ADCY1/4. We show that Ont-1/2 knockout lines have generally reduced plasma membrane/ciliary pools (except ADCY9), and total levels of cyclases, with remaining pools localized in ER. Expression of human ONT-1 rescues surface levels of cyclases in many of these lines (manuscript in preparation).

In Aim 3, we are testing the role of Ont1/2 in membrane AC/GC function. We have been characterizing the Ont-1 knockout mice. The homozygous embryos are embryonic lethal at 8.5, and exhibit complete ventralization of open neural tube (craniorachischisis), even more severe than sonic hedgehog receptor, Patched1 knockouts (separate manuscript in preparation). Strikingly, these knockouts exhibit complete reduction in total cAMP levels at E8.5 in total embryo lysates. The conditional knockouts of Ont-1 have also been generated. In comparison to Prx1Cre-Gpr161 floxed animals that exhibit extensive endochondral and intramembranous bone abnormalities (Development, 2018, PMID: 29222391), the Prx1Cre-Ont-1 floxed embryos only exhibit preaxial polydactyly, suggesting compensatory role of both Gpr161-dependent and independent pathways in regulating these skeletal phenotypes. However, CAG-Cre-ERT2-Ont-1 floxed animals are dying by 12 days of tamoxifen injection, suggesting a role of Ont-1 in cardiac physiology or metabolism. We are currently determining cause of acute death in these embryos.

CHARLES B. MULLINS, F-1436, The University of Texas at Austin. **NANO-STRUCTURED MATERIALS FOR CHEMISTRY.**

During the past grant year we have conducted experimental investigations of (1) the lithiation/de-lithiation and sodiation/de-sodiation of slurry-cast nanoparticles as well as fundamental studies of nitrogen-doped carbons as a support for lithiation-active materials such as tin, (2) advanced materials for

electrocatalysis of water reduction and oxidation, and (3) studies of the catalytic surface chemistry of gold and gold- palladium alloys. Surface chemical studies of ethanol and oxygen on gold and gold-palladium surfaces were conducted since these catalysts show great promise at low temperatures and with high selectivity. We have also searched for earth-abundant electrocatalysts for water-splitting strategies. Finally, we have continued our research regarding 3-D electrode architectures for batteries and we will have a journal article (or two) to show for this work during the next reporting period.

YUNSUN NAM, I-1851, The University of Texas Southwestern Medical Center. **STRUCTURE AND FUNCTION OF microRNA PRECURSORS.**

To determine how Drosha binds its target RNA, we are screening the ability of Drosha to process pri- miRs with variable basal junctions. We observe a range of dependence on heme for correct processing, suggesting that wild type basal junctions vary in their abilities to recruit Drosha. However, from our initial screen of pri-miRs it has been difficult to attribute Drosha binding affinity to a specific molecular feature. Thus, we are expanding our search to include more pri-miRs in our screen. In order to correlate the processing fidelity to binding affinity of Drosha, we have also tried to separate the junctions and perform in vitro binding assays using EMSA. A basal junction by nature contains two strands of RNA, and quantitative binding assays are not straightforward due to imperfect stoichiometry. Since our initial binding assays indicate that Drosha is indeed driven by binding affinity, we are also generating a library of chimeric RNAs to test how variations in the basal junction affect Drosha binding to RNA.

To determine how the apical junction of pri-miRs is recognized by the heme-binding region (HBR) of DGCR8, we are using SHAPE analysis. We have now screened more than a dozen pri-miRs using SHAPE analysis, and we observe that there is a conserved hyper-reactive site in the apical loop, centered around a nucleotide that tends to be an adenosine (Partin et al., 2017). Using mutagenesis, we are investigating the sequence and structural features that affect the SHAPE signal. We have determined that the stem-loop structure is vital for recognition by HBR, and will continue to identify more molecular features.

How heme can switch on the ability of DGCR8 to recognize the terminal loop is unknown. We have used electron microscopy to show that DGCR8-Drosha complex undergoes a major conformational change upon binding heme. We are screening various truncation constructs of HBR, to determine the structural basis for the ability of heme to activate DGCR8.

DOUGLAS NATELSON, C-1636, Rice University. **NOVEL SINGLE- AND FEW-MOLECULE VIBRATIONAL SPECTROSCOPIES.**

In the last year, we have continued to make good progress toward our goals. Through quantifying optical heating in our nanostructures, we had discovered unexpected spatial variations in the thermoelectric response of polycrystalline metal films, work now published in the RSC journal *Nanoscale*. This has spawned follow-on experiments to understand the mechanism at work, employing single-crystal nanowires made by collaborators from Stanford. This work will be submitted for publication in August. In related work, we have found that oxygen plasma exposure of Au nanowires can create a AuOx coating, that the 785 nm laser drives decomposition of the AuOx, that this decomposition is not simply thermal, and that the Au/AuOx junction can be detected via its large photothermoelectric response. This demonstrates both that surface chemistry can alter thermoelectric response, and that photothermoelectric measurements can detect surface photochemistry on nanostructured substrates. This work is also going to be submitted shortly.

Directly relevant to the goal of simultaneous Raman and electronic spectroscopy, we have been designing substrates for remote excitation of propagating surface plasmon polaritons (SPPs) that deliver optical energy to the nanojunctions. This mitigates direct optical heating of the junction. Bolometric conductance measurements, to detect temperature changes of the junction, have demonstrated that this approach delivers energy to the junction while cutting the local temperature increase by a factor of 60 compared to direct illumination. This work has been published in *Nano Lett*. In bare nanogaps, we have found that hot electrons can be generated and hot electron photocurrents can be driven by the remotely excited SPPs. Initial results have been published in a SPIE conference proceeding, and a detailed write-up is in preparation. We are now in the process of attempting single-molecule Raman measurements via this remote excitation approach.

DONALD G. NAUGLE, A-0514, Texas A&M University. **THE INFLUENCE OF REDUCED DIMENSIONALITY, DISORDER, AND INTERFACES ON THE PROPERTIES OF SOLIDS.**

We have refurbished our UHV low temperature deposition cryostat to investigate effects of decoration of monolayer/submonolayer adatoms onto the surface of mono- and bi-layer graphene. Dilute ($n < 5 \times 10^{12} \text{ cm}^{-2}$) alkali (K, Li) adatom decoration of both mono- and bi-layer graphene in a FET configuration at $T=20\text{K}$ was accomplished. The decorated graphene was characterized by electrical conductance measurements as a function of gate voltage V^G between graphene and a SiO₂/Si substrate from 20K to 2K, from 2K to 300K during annealing, and then on cooling back to 2K. The Dirac (charge neutrality) point at $V^G = V^D$ provides direct measure of electron transfer from K(Li) to the graphene. The temperature dependence of V^D for both Li and K decorated monolayer and bilayer graphene indicates that the adatoms are mobile on graphene for $T > 30\text{K}$ and begin to form clusters during annealing, in agreement with our DFT calculations. For monolayer graphene doped with surface alkali adatoms the electronic charge carrier mobility is dominated by scattering from the charged adatoms. Study of K adatoms on bilayer graphene in this concentration regime shows that two factors control electrical transport in the presence of these adatoms, the Thomas-Fermi screening length and the adatom impurity charge concentration, n , in agreement with Boltzmann transport theory. Our (APL) paper on K adatoms on monolayer graphene was highlighted in AIP "Scilight": J. H. Majors, "Diffusion of alkali metal adatoms decorated on graphene dominates its electrical response", <https://doi.org/10.1063/1.5020508>. Other efforts this period also included: development and characterization of new wear resistant multiphase decagonal quasicrystal alloys and detailed description of approaches to fabrication of the nanostructures used in our Welch supported previous studies of the interplay of superconductivity and magnetism at the nanoscale that we have published over the past few years.

ANDRIY NEVIDOMSKYY, C-1818, Rice University. MULTIPOLAR SPIN ORDERS IN CORRELATED ELECTRON MATERIALS.

Nevidomskyy's group efforts have concentrated on two major research directions. One, on the multipolar spin order in frustrated magnets, has its foundation in the Phys. Rev. Lett. article in 2016. This research has continued in a recently published Phys. Rev. B paper proposing a unified theoretical model to explain the properties of Fe(Se,Te) family. We have further performed a state-of-the-art study of a frustrated spin-1 model on a square lattice, applicable to FeSe and other materials, with the intriguing result that a new class of quantum spin liquid (QSL) is realized (submitted to Phys. Rev. Lett, arXiv:1711.06523). QSLs are strongly entangled quantum phases whose existence has long been proposed (going back to Anderson's RVB), but an unambiguous experimental realization of which is yet to be found. The PI's work in search for QSLs has resulted in another two papers, one of which has been submitted to Science and is devoted to the use of quantum entanglement probes in search of QSLs. In a related work that is about to appear in Nature Commun, the PI has teamed up with Rice colleague Pengcheng Dai to understand the interplay of magnetism and the orthorhombic lattice distortion in the Ni-doped iron pnictide NaFeAs. The second thrust focuses on the role of topology in magnets and superconductors alike, which has become subject of intense research recently. The PI has submitted three manuscripts on the subject, of which I would especially like to highlight the work on topological superconductivity performed in collaboration with Matthew Foster (arXiv:1708.07825). In this monumental 40+ page paper, we have performed an exhaustive analysis of the role that topology plays in superconductivity in cubic lattice materials, particularly relevant to the half-Heusler family of compounds. In addition to the above main thrusts, the grant also supports efforts studying the Mott metal insulator transition and the Kondo lattice materials (1 article published and 4 submitted).

KYRIACOS C. NICOLAOU, C-1819, Rice University. TOTAL SYNTHESIS OF BIOACTIVE NATURAL AND DESIGNED MOLECULES.

1. Completed a collaborative study with the Shamoo group that led to the evolution of diverse strains as a method for the determination of biochemical mechanisms of action of novel pyrrolizidinone antibiotics (publication in ACS Infect. Dis.).
2. Developed improved total syntheses of several naturally occurring trioxacarcins and numerous designed analogues and subjected them to biological evaluation with regards to their antitumor properties (publication in JACS).
3. Completed our synthetic work on antibiotic CJ-16, 264 and its analogues and their evaluation that led to a number of potent and yet simpler than the parent compound (publication in JACS).
4. Completed the first total syntheses of the tubulin binding natural products disorazoles A1 and B1, and assigned the structure of the latter (publication in JACS).
5. Published an invited extensive review titled, "A Brief History of Antibiotics and Select Advances in Their Synthesis" from our group (published in J. Antibiotics).
6. Published an invited Essay titled, "The Emergence and Evolution of Organic Synthesis and Why It is Important to Sustain It as an Advancing Art and Science for Its Own Sake" (published in Isr. J. Chem).
7. Synthesized a number of natural and designed tubulysins and subjected them to biological evaluation leading to the discovery a number possessing extreme potencies against tumor cells (publication in JACS). A number of these and other compounds from the ones mentioned above are currently advancing as payloads on antibody-drug conjugates as preclinical candidates.

DEEPAK NIJHAWAN, I-1879, The University of Texas Southwestern Medical Center. EXPANDING THE DRUGGABLE GENOME.

We have previously identified the mechanism of action for the anticancer sulfonamide. Indisulam has a novel mechanism of action – it recruits the splicing factor, RBM39, to the E3 ubiquitin ligase DCAF15, resulting in RBM39 poly-ubiquitination and proteasome mediated degradation. We aim to identify novel small molecules that also act by recruiting neo-substrates to E3 ubiquitin ligases. We previously identified 2,700 by performing a high throughput small molecule screen of 200,000 compounds. In the past year, we have developed a CRISPR/Cas9 based screen to determine whether the activity of an anticancer compound is dependent on an E3 ubiquitin ligase. In brief, we have synthesized a CRISPR/Cas9 library containing ~4000 guide RNA's designed to target ~649 E3 ubiquitin ligases. This library is stably expressed in cells that are treated with novel compounds identified in our screen. Two weeks following treatment, the barcoded guide RNA's are amplified from the cells and analyzed for enrichment of specific guides. Using this screen, we identified components of the DCAF15 complex in cells that were treated with indisulam. This result serves as a positive control for the screen. We are now applying this screen to each of the 2,700 compounds with anticancer activity in our small molecule screen.

MICHAEL NIPPE, A-1880, Texas A&M University. SYNTHETIC STRATEGIES FOR THE PREPARATION OF SUPRAMOLECULAR AND COVALENT CAGE STRUCTURES CONTAINING CARBORANE MOIETIES.

Thanks to the financial support through this grant, we were able to make important discoveries in several areas. In the area of electrocatalysis we reported the first example of an imidazolium-functionalized molecular catalyst that displayed significantly improved catalytic metrics (J. Am. Chem. Soc.). In the area of structure and bonding, we disclosed the first experimental and computational comparative studies of Dy-Fe and Dy-Ru bonded complexes (Angew. Chem. Int. Ed.). In the area of single-molecule magnetism, we reported on unusually strong ferromagnetic coupling in multinuclear lanthanide ferrocenophane chain complexes (J. Am. Chem. Soc.) which results in well-defined magnetic hysteresis curves with significant remnant magnetization at zero field. We also disclosed a comparative magnetic, structural, and computational study of mononuclear Tb and Dy ferrocenophane complexes (Angew. Chem. Int. Ed.), and discovered important similarities between our newly discovered ferrocenophane complexes and the iconic lanthanide bis-phthalocyanine complexes. These important results are guiding our future molecular design principles for high performance SMMs. We also published a unique set of lanthanide complexes that in which the magnetic relaxation times of the lanthanide ion can be switched reversibly as a function of oxidation state of a nearby transition metal ion (Chem.

Sci.). This was only the second report of using transition metal redox changes to alter magnetization dynamics of a lanthanide ion. Importantly, our molecular design allows for much more chemical stability of the molecules in various oxidation states while previous examples suffered from thermal instability.

QIAN NIU, F-1255, The University of Texas at Austin. **PROPERTIES AND THEIR INTER-COUPPLINGS IN 2D MATERIALS.**

We have studied inter-couplings of electronic and magnetic degrees of freedom, focusing on disorder effects in the so-called spin-orbit torques, which have been found to be important in spintronics applications. We have published two articles considering both the weak-disorder Boltzmann limit and beyond. We have also studied topological phase transitions in thin films by tuning multivalley boundary-state couplings. In addition, we re-examined the classic problem of Landau level quantization by successively including magnetic response functions, such as zero-field magnetization and susceptibility. Our theory not only reproduces Onsager's rule at zeroth order and the Berry phase and magnetic moment correction at first order, but also explains the nature of higher-order corrections in a universal way.

PETER J.A. NORDLANDER, C-1222, Rice University. **THEORETICAL INVESTIGATIONS OF CHEMICAL PROPERTIES OF NANOSYSTEMS.**

We have continued our progress on the development of aluminum as a sustainable material for plasmonics and light harvesting applications. Notable successes include a novel chemical approach for synthesis of aluminum nanorods with tunable plasmonic properties, the development of an aluminum-based plasmonic pixel with active and reversible full-spectrum tunability and a demonstration that aluminum nanocrystals can be used for quantitative surface enhanced Raman scattering-based DNA detection. In the area of plasmon induced photocatalysis, we have developed an approach for chemical synthesis of transition-metal decorated aluminum nanocrystals that can serve as efficient antenna-reactor structures. Our progress in the area of quantum and molecular plasmonics includes the development of a novel theoretical method for identifying and characterizing emerging plasmonic behavior in small clusters and molecules. We have also developed a fully quantum mechanical method for the description of hot carrier relaxation. This approach provides a quantitative description of the carrier relaxation process including electron-electron scattering, photoluminescence and photothermal heating. In this context we have also studied the damping of plasmon-induced acoustic oscillations in plasmonic molecules. We have also begun an exploration of plasmon induced photothermal effects in applications such as remote heating, photocatalysis, and photodetection. In the area of plasmon enhanced imaging and spectroscopy, we have shown that photoinduced force microscopy can be used for precise imaging of heterometallic antenna-reactor structures, developed efficient plasmonic aluminum and gold antennas for ultrasensitive surface enhanced infrared absorption spectroscopy, and also investigated how environmental symmetry breaking can lift the degeneracy of dipolar plasmon modes in nanotriangles.

SIMON W. NORTH, A-1405, Texas A&M University. **FUNDAMENTAL IMAGING STUDIES OF CHEMICAL REACTIVITY.**

We recently published a method to extract speed-dependent vector correlations from sliced ion images to include 2+1 REMPI detection. We continue to work in collaboration with Dr. Wei Wei on extending this approach to alternative polarization geometries which should provide greater sensitivity to the underlying stereodynamics. Our results enable a broader application of the imaging technique to a wider range of chemical systems. In particular, in the case of O₃ photodissociation we have identified the mechanism responsible for the interesting odd rotational state suppression in the O₂ products first observed by Valentini and co-workers over 30 years ago. Our first manuscript on this system involving new high resolution measurements and classical trajectory calculations in collaboration with Dr. George McBane has been submitted to the Journal of Chemical Physics. We are currently finishing ion imaging measurements and analysis to confirm our hypothesis that O₃ photodissociation produces O₂ products with a strong preference for a single lambda doublet preference, similar to the behavior observed in our previous study of NO₃ photodissociation. This refutes earlier work which implicated O₃ photodissociation as a mechanism for strong isotopic fractionation in the atmosphere. We have made considerable progress on the study of the photodissociation of benchmark systems CH₂O and CH₃CHO using a newly acquired and modified ion imaging instrument to establish a connection between the measurement of photofragment vector correlations in roaming systems and the nature of abstraction transition states and ultimately the dynamics of radical-radical bimolecular reactions with an unprecedented level of detail. A manuscript describing our work on CH₃CHO system will be submitted by the end of the year.

KATHRYN A. O'DONNELL, I-1881, The University of Texas Southwestern Medical Center. **DISSECTING NOVEL MECHANISMS OF LUNG CANCER PATHOGENESIS.**

The purpose of AIM 1 is to elucidate the mechanisms through which PCDH7 promotes tumorigenesis and identify the key mediators that connect PCDH7 to the MAPK pathway. In human bronchial epithelial cells and NSCLC cell lines, PCDH7 overexpression synergizes with KRAS and EGFR to induce MAPK signaling and tumorigenesis. Conversely, PCDH7 depletion suppresses ERK activation, sensitizes cells to MEK inhibitors, and reduces growth of NSCLC xenografts. We demonstrated that these oncogenic effects are associated with the ability of PCDH7 to bind to Protein Phosphatase 2A (PP2A), which directly de-phosphorylates ERK1/2, and the SET oncoprotein, a potent inhibitor of PP2A, thereby suppressing PP2A activity. Collectively, this work uncovers a new mechanism through which PCDH7 leads to hyperactivation of the MAPK pathway, a critical driver of lung tumorigenesis (Zhou et al, Cancer Research, 2017).

The purpose of AIM 2 is to develop a PCDH7 neutralizing antibody and test the therapeutic efficacy in a mouse model. We were successful in expressing the extracellular domain of PCDH7 in insect cells with greater than 90% purity at high concentrations. We set up a collaboration with Dr. Zhiqiang An, (UT Health Science Center at Houston), who leads a Therapeutic Monoclonal Antibody Lead Optimization and Development Core. We have worked with

Dr. An to develop antibodies using 1) scFv phage display 2) and rabbit immunization to generate individual B cell culture supernatants. We generated the following: 131 rabbit B cell culture supernatants from rabbit immunization and 30 PCDH7 antibody candidates from phage panning. For the phage display approach, 387 phages were sequenced and tested for ELISA- based binding to PCDH7, which yielded 30 unique candidates. In the coming months, we will evaluate antibody candidates for their ability to block PCDH7 function. We plan test the therapeutic efficacy of these antibodies in immunocompromised mice harboring patient-derived NSCLC xenografts.

JOHN S. OLSON, C-0612, Rice University. CHEMICAL MECHANISMS OF LIGAND BINDING TO HEME PROTEINS.

During the four-month no-cost extension, we completed our study of the assembly of adult human hemoglobin (HbA) and applied some of the ideas to the engineering of more stable hemoglobin-based oxygen carriers in two new papers that have just been published on line. The mechanism for human Hb folding and heme association is similar to that for Mb. The initial step is the transient folding of alpha and beta monomers and then to form a dimeric apoHb dimer intermediate in which the heme pockets are melted but the helices at the N and C terminal regions of both subunits are stabilized by extensive favorable hydrophobic interactions in the alpha1beta1 dimer interface. The final, major pathway involves folding of the heme pocket, high affinity binding of heme, and association of the holoHb dimers into native and fully functional tetramers. However, heme can also bind to the molten dimeric intermediate, albeit weakly, to generate a reversible hemichrome intermediate which folds rapidly into a native holo-Hb dimer. Premila P. Samuel (Mohan Dass), a Welch Predoctoral Fellow performed these studies, and she defended her thesis on October 13, 2017. The detailed analysis of holoHb unfolding and verification of the proposed mechanism will be part of final publication acknowledging Welch Foundation support.

MOHAMMAD A. OMARY, B-1542, University of North Texas. DAWN RISE UPON NEW CHEMICAL BONDS AMIDST GROUND- AND EXCITED-STATE BONDING ASSORTMENTS IN LUMINESCENT MOLECULES/EXCITONS/POLARONS.

Notable results toward each objective:

(A) A posteriori and a priori discoveries of counterintuitive covalent M-M' and M-M in bridge-dimeric systems of monovalent d10 coinage metals with S^ΛC asymmetric ligands: Mixing of (n+1)s₀/p₀ orbitals with (n)d₁₀ orbitals was responsible for polar-covalency, manifesting ds' and dp' interatomic hybrid orbitals. [Otten et al., *Comments Inorg. Chem.* 2018, 38, 1–35.]

(B) In situ synthesis for a phosphorescent heavy-metal-ion sensor, [Au(3-CH₃,5-COOH)Pz]₃, (aka Au3Pz3) in aqueous chitosan polymer media: Au3Pz3 exhibits red emission (max ~690 nm) but addition of silver salt attains green emission at 475–515 nm due to cation-p adduct (Ag⁺@Au3Pz3) formation. With almost zero interference from 15 other metal ions tested, Au3Pz3 exhibits extreme selectivity for Ag⁺ with ppb/nM detection limits. Au3Pz3 exhibits sensitivity to higher concentrations (> 1 mM) of several other metal ions (Tl⁺/Pb²⁺/Gd³⁺) due to formation of their corresponding cation-p adducts akin to the Ag⁺ analogue. [Upadhyay et al., *Anal. Chem.* 2018, 90, 4999–5006.]

(C) Stacked [Au₃(RN=CR)₃]_n complexes in various conformations were studied computationally at the MP2 and DFT levels. Structure optimizations yielded the lowest energy for a slided stacked (parallel- offset) conformation of [Au₃(HN=COH)₃]₂, yet unrealized experimentally. Per MP2, the slided conformer is 32 kJ/mol more stable than staggered, which in turn is 11 kJ/mol below eclipsed -- due to greater multipolar interactions in the former whereby the most p-basic and most p-acidic quadrupolar regions of adjacent cyclotrimers are lined up. Per DFT, aromatic ligands lead to a planar/prismatic structure of [Au₃(PhN=COMe)₃]₄ vs chair conformation for for [Au₃(cPeN=COMe)₃]₄. Photophysics modeling reproduces experimental trends, with large Stokes shifts due to metallophilic-to-excimeric bonding transformation upon photoexcitation. [Rabaa[^] et al., *Inorg. Chem.* 2018, 57, 718-730.]

JOSÉ ONUCHIC, C-1792, Rice University. INTEGRATING STRUCTURAL AND CO-EVOLUTIONARY GENOMIC DATA TO DETERMINE THE ENERGY LANDSCAPE OF BIOMOLECULAR COMPLEXES.

The combination of structure based models (SBMs) and direct coupling analysis (DCA) infers physical contacts in a protein or protein complex. This year we continued to use our integrated computational framework called fragment docking and DCA analysis (Fd-DCA) to understand how drugs such as the mitocan cluvanone alter the stability of NAF-1 and mitoNEET clusters and affect the growth of breast cancer cells in culture. In addition, we generalized our DCA coevolutionary landscape to make predictions of single amino acid substitutions that produce functional interactions between non-cognate, interspecies signaling partner proteins. Specifically, predictions of phosphotransfer activity between the Escherichia coli histidine kinase EnvZ to the non-cognate receiver Spo0F from Bacillus subtilis were compiled and confirmed experimentally (manuscript is in preparation).

Our Minimal Chromatin Model (MiChroM) explains the folding of interphase chromosomes and generates chromosome conformations consistent with experiments (last year report). The energy landscape of the model relies on two experimentally derived inputs: a classification of loci into chromatin types and the positions of chromatin loops. To overcome the need for these experimental inputs, we have developed a model, called the Maximum Entropy Genomic Annotation from Biomarkers Associated to Structural Ensembles (MEGABASE), where chromatin architecture can be predicted de novo using epigenetic data derived from chromatin immunoprecipitation-sequencing (ChIP-Seq). We validated the predicted structural ensembles by using ChIP-Seq tracks alone to predict Hi-C maps, as well as distances measured using 3D fluorescence in situ hybridization (FISH) experiments. The results support the hypothesis of phase separation being the driving process behind compartmentalization. These findings strongly suggest that epigenetic marking patterns encode sufficient information to determine the global architecture of chromosomes.

KIM ORTH, I-1561, The University of Texas Southwestern Medical Center. USING CHEMISTRY AND GENETICS WITH VopQ TO DECIPHER VACUOLAR FUSION EVENTS.

Over the last year we have analyzed the inhibitory properties of VopQ. Based on our 2017 Science Signaling paper showing that the *Vibrio T3SS1* rewires host gene expression to subvert cell death and activate cell survival pathways, we asked what role does VopQ play in manipulating these signaling pathways. By analyzing the transcriptional response of the host cell infected with bacterial expressing VopQ or deleted for VopQ, we demonstrated that VopQ is the primary driver for inducing the survival signals in the host cell via a MAPK dependent mechanism. Using a mutant of VopQ (P200S) that can make pores but no longer inhibit vesicular fusion, we further show MAPK signaling is generated from an ancient signaling pathway using the ER stress receptor Ire1. Here we observe that VopQ-mediated blockage of autophagic flux can induce the clustering, phosphorylation and activation of Ire1 in both yeast cells and mammalian cells. As these findings reveal a new line of communication between autophagy and ER stress sensors, we are preparing a manuscript for a high-profile journal.

In preparation for our cryo-EM studies with VopQ and the lysosomal V-ATPase, we have isolated a bacterial toxin ClyA from *E. coli* to use as test protein for this experimental platform. We have been successful in isolating this toxin and showing that the ClyA pore complex can exist as dodecamer, tridecamer or tetradecamer. The resolutions for the three different oligomers are 2.8 Å, 3.2 Å and 4.3 Å, respectively. Additionally, we observe with negative staining the ClyA forms a soluble intermediate state, likely to be a trimer. We are completing further biochemical analysis if this pore forming toxin and plan to write up our finding in a manuscript to submit to a structure journal in short order. Now that we have a successful knowledge base for using the Cryo EM facilities at UT Southwestern. We will move on with our goal of solving the soluble and membrane bound structures of VopQ.

OLEG V. OZEROV, A-1717, Texas A&M University. LIGAND DESIGN APPROACHES TO COUPLING CATALYSIS WITH GROUP 9 METAL COMPLEXES.

Our approach to the development of new rhodium and cobalt catalysts for coupling reactions relies on controlling the reactivity at the metal center using modifications of the supporting ligands. We utilize the pincer-type ligands to provide access to 3-coordinate, unsaturated, low-valent Rh or Co species. Our research thus combines design and general studies of new ligands and studies of coupling-related reactivity of their Rh and Co complexes.

Previously, we established that POCOP and the related aryl-centered ligands are not suitable for Co catalysis because of the undesirable coupling between the aryl of the pincer ligand and the aryl of the aryl halide reagent. In the past year, we continued exploring the use of PNP ligands which do not undergo N- C coupling with the pincer ligand nitrogen. We have been able to establish that C-S reductive elimination is possible without affecting the supporting PNP ligand, but the catalysis is thwarted by the comproportionation of the Co(I) and Co(III) intermediates to the undesired Co(II) products. We have explored the fundamental chemistry of this comproportionation and are now designing new systems that should avoid the comproportionation obstacle. We have also developed a better understanding of the synthetic chemistry of the introduction of Co into pincer complexes. Most recently, we discovered that (PNP)Co systems are capable of cleavage of C-O bonds in aryl carboxylates, opening up possibilities for the utilization of these advantageous substrates in Co-based coupling catalysis.

Our general work on the exploration of the properties of pincer ligands led to a discovery of reversible dearomatization of a common PCP ligand. The analogous dearomatization of the isoelectronic pyridine- based PNP ligands is well established in the literature and is key to a suite of catalytic reactions. The discovery of the analogous chemistry with the aryl-centered PCP ligand may lead to new catalytic applications.

JEREMY C. PALMER, E-1882, University of Houston. METASTABLE LIQUID-LIQUID PHASE TRANSITIONS IN MOLECULAR MODELS OF TETRAHEDRAL FLUIDS.

Anomalous scattering in water and silica. We performed large scale molecular dynamics simulations of systems > 32,000 molecules of the ST2 water model [Mol. Phys. 15-16, 1953-1964, 2018] and the mWAC silica model to investigate their low-temperature scattering behavior. Our previous studies demonstrated that both models exhibit LLPTs under deeply supercooled conditions. Our analysis reveals the presence of highly coupled, long-wavelength fluctuations in density and local tetrahedral order in both supercooled liquids. In both models, these fluctuations increase dramatically upon cooling and give rise to anomalous small-angle scattering, reminiscent of that observed in experiments on supercooled water. We also find that the static correlation length associated with these fluctuations diverges upon cooling, consistent with the presence of a critical singularity. We anticipate that these results will be of use in interpreting recent scattering experiments on supercooled water [e.g., Kim et al., Science 385, 1589- 1593, 2017].

Effect of confinement on LLPTs. We used simulation to investigate the effects of confinement in nm-sized pores on the LLPT in the mWAC silica model. Numerous experiments have been performed on water in confinement to stabilize the liquid against crystallization under deeply supercooled conditions. Unfortunately, the phase behavior of confined systems cannot be straightforwardly related to those of bulk liquids. Our study reveals that confinement suppresses mWAC's LLPT by shifting it to lower temperatures; the liquid-liquid critical temperature decreases monotonically with increasing confinement. We find that this suppression occurs in both hydrophobic and hydrophilic nanopores. This key finding suggests that experiments on water must be performed at significantly deeper supercoolings to search for an LLPT. We are currently working on a manuscript to report the results from this study.

KEITH H. PANNELL, AH-0546, The University of Texas at El Paso. SILOXYMETHYLAMINES: MASKED AMINATION REAGENTS FOR NEW METAL LIGANDS.

The potential of Et₃SiO-CH₂NMe₂, 1, as a Mannich aminomethyl transfer agent has continued with studies elucidating its reactions with a series of anilines, (p-RC₆H₄)NH₂. The parent aniline, R = H, initially led to formation of the triamine (p-RC₆H₄)N(Me₂NCH₂)₂ which was observed as a transient

only by NMR spectroscopy. Attempts to isolate this material failed and led to high yield isolation of hexahydro-2,4,6-triphenylamino-1,3,5-triazine, (PhNCH₂)₃. Changing the R group substituent on the starting aniline was dramatic. In the case of electron-donating groups Me₂N and MeO the reaction was instantaneous to form the corresponding triazine. In contrast, the electron-withdrawing substituent CF₃ resulted in the high yield formation, and isolation of the diamine (p-CF₃-C₆H₄)NHCH₂NMe₂. Further reaction with 1 led to high yields of the triamine (p-CF₃-C₆H₄)N(CH₂NMe₂). Both the diamine and triamine were characterized by single crystal XRD and are among the very few examples of such materials where the N atoms are separated by a methylene group and indeed the first to be structurally characterized diffraction. In neither case was any triazine formation observed. Use of the bulky aniline (2,6-Ph₂CH)-4-tBu-C₆H₃)NH₂, R'NH₂, resulted in the immediate and sole formation of the corresponding imine R'N=CH₂, which was characterized via single crystal XRD, only the second such example.

Thus, the sequence of reactivity of anilines (p-RC₆H₄)NH₂ with 1 has permitted us to observe, isolate and structurally characterize, for the first time, each step in the process, aniline diamine (R = CF₃) triamine (R = CF₃) imine (R = 2,6-(Ph₂CH)₂-4-tBu-C₆H₂) triazine (R = NMe₂, OMe), dependent upon the electronic impact of aniline substituents.

The synthesis of new organolead materials of the type Ph₂(Ar)PbCl and Ph(Ar)PbCl₂, [Ar = o- MeECH₂-C₆H₄, E = O and S] has been accomplished. Single crystal X-ray analysis indicates very strong intramolecular E...Pb interactions. The presence of this bonding motif is reflected in the chemistry of aryl group transfer to tin halides where only Ph transfer occurs.

Our study on the formation of 8-amido-BODIPYs from 8-amino-BODIPY precursors has been completed. Empirically modified DFT calculations were shown to accurately predict the optical absorption of the materials and also predicted that the LUMO of the systems was anti-bonding with respect to the N-C8 bond. This latter result suggests that simple photochemical radiation into the HOMO to LUMO band gap will result in new substitution chemistry.

MATTEO PASQUALI, C-1668, Rice University. PHYSICAL CHEMISTRY OF NANORODS AND NANOPATES.

We continue to use carbon nanotubes (CNTs) as model system to study the fundamental behavior of solutions and colloidal dispersions of nanoparticles. We study the behavior of very long CNTs formed via the floating catalyst method combined with continuous drawing out of the synthesis furnace. We find that purification is key to controlling dissolution and liquid crystal formation for these CNTs, and that their length (below 50 m) is lower than previously believed (with Duong). We investigate doping in CNT fibers and find that iodine forms chains that intercalate both inside the CNTs as well as in the interstices between CNTs; we find that, by selective de-doping fiber sections, we can make weavable photodetectors (with Puech & Kono). We study the composition of boron nitride nanotube (BNNT) samples produced by laser vaporization; we find that more than 50% of the material comprises hexagonal boron nitride (hBN). By cryo-TEM, we find that the purified BNNT dissolves spontaneously in strong acids and that dissolution can be used to extract small quantities of high-purity BNNTs from mixed BNNT/hBN samples. These purified BNNTs can form self-standing macroscale films and aerogels (with Talmon). By exploiting CNT fluid phase behavior, we develop a novel method to make well-aligned, packed CNT fibrils with mg quantities of material, 100x lower than previous methods. We show that CNT fibril conductivity and strength scale linearly with CNT aspect ratio and that better packing in CNT fibrils leads to 2x strength than previously determined via solution-spun fibers. By understanding the interactions of CNTs with acids and surfactants and the effect of these interactions on CNT phase behavior, we use dialysis to form high-concentration CNT liquid crystals in water with minimal sonication and CNT damage. We form highly oriented macroscale CNT fibers and show that the strength of these fibers is comparable to CNT fibers spun from acid solvents, while conductivity remains lower.

MARGARET A. PHILLIPS, I-1257, The University of Texas Southwestern Medical Center. PURINE SALVAGE PATHWAYS AS POTENTIAL DRUG TARGETS IN TRYPANOSOMATID PARASITES.

We have already demonstrated and published on the essentiality of GMP synthase. In the past fund year we have been working to complete genetic knockout studies on adenylosuccinate lyase (ADSL). We have found the gene to be essential and we are just completing metabolomics analysis of the knockout cell lines to further understand the metabolic deficiencies that result from perturbing this pathway. We expect to write up a manuscript on this work in the next 6 months. As a prelude to developing high throughput assay strategies to evaluate the purine biosynthetic genes, we have been working to develop methods to assay multiple trypanosomatid species enzymes simultaneously. As a proof of concept we have been using *T. brucei* thymidine kinase (TK) and we are developing a yeast based growth assay that would allow *T. brucei*, *T. cruzi*, *Leishmania* TK to be evaluated in a single screen. We have also expanded our program to evaluate the role of nucleotidases in both the purine and pyrimidine metabolic pathways so we can understand their role in regulating pathway flux. We previously showed that the essentiality of TK was due to the presence of nucleotidases in *T. brucei*. We identified three strong gene candidates that might encode this activity and we showed that one of these candidates did encode an active nucleotidase. We are in the process of generating recombinant enzymes for the remaining two nucleotidase candidates, and we are evaluating the roles of these candidate genes on parasite growth and on purine and pyrimidine biosynthesis by generating knockouts. These studies will help us to prioritize the best enzyme candidates in these pathways for drug discovery by fully understanding what enzymes control flux in the pathway.

LIONEL W. POIRIER, D-1523, Texas Tech University. NEW METHODOLOGIES FOR ACCURATE QUANTUM CALCULATIONS OF THE DYNAMICS OF ATOMIC NUCLEI.

The proposal for this grant outlined the following 3 areas for the 2016-2019 grant cycle: 1) phase space basis set methods; 2) quantum trajectory methods; 3) rovibrational state labeling technology. In the last year, significant progress has been made in all three areas, leading to a total of five published

articles acknowledging Welch support. Note that the state of Texas will not deliver TRIP match support this coming year, but the recent \$10,000 Welch supplement will be used to make up the difference.

Regarding 1), in addition to the Adv. Chem. Phys. book chapter having been published [note: publisher does not allow uploads] our application of this technology to electronic structure & dynamics [work by postdoc J. Jerke] led to the fourth-most read JCP article in March 2018 [JCP 104101 (2018)], a talk at the University of Chicago, and an invitation to attend a Gordon Research Conference. Also, the robust basis-finding algorithm (described in the proposal) was applied to OCHCO+, leading to an MS thesis, and an upcoming JCP submission. An unexpected by-product of this technology is its use as an efficient potential surface “hole finder”, which will be explored going forward.

Regarding 2), the application to quantum capture probabilities for complex-forming reactions in molecular astrophysics has led to a recent JCP Communication [JCP 021101 (2018)] and several talks, plus several collaborations including my present sabbatical at the Max Planck Institute, and the recent MPI-funded “Focus Workshop on Quantum and Semiclassical Trajectories” which I organized.

Regarding 3), this work has led to two additional published articles, as well as two upcoming articles (in preparation) that examine the fundamental rotation-vibration problem in molecular spectroscopy from a new perspective. Over the last 12 months, Welch-supported projects have led to 15 invited, mostly international oral presentations, including a high-profile talk at the famed Perimeter Institute.

DAVID C. POWERS, A-1907, Texas A&M University. PCET-TRIGGERED METAL-LIGAND COOPERATION FOR AEROBIC OXIDATION CATALYSIS.

Our research efforts to develop new platforms for sustainable oxidation chemistry has progressed along two complementary lines of investigation:

1. We have developed aerobic oxidation of aryl iodides to generate families of hypervalent iodine reagents, which were targeted because they are widely used selective oxidants in organic synthesis. We achieved aerobic oxidation by diverting reactive oxidants generated during aldehyde autoxidation towards the oxidation of aryl iodides. The developed aerobic oxidation conditions have been applied to oxygenation, amination, and halogenation reactions. We extended these efforts to an aerobically generated Dess-Martin Periodinane analogue, which enabled aerobic alcohol and amine oxidation reactions. These efforts have resulted in publications in Nature Chemistry and Angewandte Chemie.

2. In a complementary effort, we developed new experimental tools to examine the mobility of liquid-phase substrates inside porous catalyst materials. This work was motivated by the need to understand substrate mobility in order to leverage matrix confinement of hydrocarbons as a strategy to realize selective intermolecular C–H oxidation chemistry. Using kinetic isotope effect measurements developed in enzymology, we demonstrated direct evaluation of the relative rates of substrate oxidation and catalyst turnover. This work resulted in a publication in Angewandte Chemie.

3. We have continued our efforts to develop new chemistry and techniques to characterize reactive intermediates in C–H oxidation. During the previous year of this funding cycle, we characterized a reactive Ru₂ nitrido by photocrystallography. During this year, we have extended these efforts to the characterization of a reactive Rh₂ nitrenoid, which is a critical intermediate in widely utilized Rh₂-catalyzed C–H oxidation. This work has resulted in a publication in revision at the Journal of the American Chemical Society.

B. V. VENKATARAM PRASAD, Q-1279, Baylor College of Medicine. X-RAY CRYSTALLOGRAPHIC STUDIES ON VIRUSES AND VIRAL PROTEINS.

During 2017-2018, we have made exciting progress toward the proposed aims and discovered novel features. Our structural studies are related to three medically important viruses: Rotaviruses, major pathogens of infantile gastroenteritis; Noroviruses, which cause epidemic diarrhea in humans; and Influenza viruses, which cause seasonal and pandemic flu. In regard to rotaviruses: (1) we determined the structural basis of glycan specificity in globally-dominant rotavirus strains belonging to P[6], P[4] and P[8] genotypes, and showed that they exhibit a novel binding site and allowed to propose the structural basis of their global dominance, and why some P[6] strains are neonate specific (Hu et al., 2018, Nature Commun); and (2) we provided a structural rationale for how a novel phosphorylation cascade alters NSP2 oligomerization and suggested how that may be an important factor for regulating viroplasm formation (Criglar et al., 2017, manuscript in review in PNAS). (3) We determined the first structure rotavirus capping enzyme VP3 to 2.7 Å resolution using single-particle cryo-EM techniques (Kumar et al., manuscript in preparation). In regard to noroviruses, (1) we determined the first crystallographic structure of the protease encoded by GI.4 noroviruses, which are the globally most prevalent norovirus strains. This study showed several novel differential features compared to GI proteases and provided a structural rationale for a novel pH-sensitivity to this protease (Viskowska et al., 2017, Manuscript being submitted). We also have now initiated high-throughput screening of small molecule inhibitors for norovirus proteases. In regard to influenza virus, we have carried out the several crystal structures of the NS1 mutants that allow us to understand how structural plasticity affect its function (Mitra et al., Manuscript in preparation).

HAN PU, C-1669, Rice University. SYNTHETIC P-WAVE INTERACTION IN ULTRACOLD ATOMS.

Tuning the two-body interaction between two atoms in the ultracold temperature regime is now a mature technique in the field of cold atoms. During this past year, we continue to investigate the fundamental properties of cold atomic ensembles in both the few- and many-body regimes. We have proposed a novel method to generate spin-orbit coupling (SOC) in a mixture of spinor quantum gases. The key is to apply Raman beams to one species in the mixture, which generate the standard SOC in that species, and then through the inter-species spin exchange interaction, the effect of SOC can be transferred to the other species in the mixture. This provides a unique opportunity to study SOC in superfluid mixtures which is almost impossible to realize in solid state systems. We have developed a powerful theoretical technique to construct the wavefunction, and to calculate the momentum distribution, of a spinor quantum gas confined in one dimension (1D) in the strongly interacting regime. This system exhibit many intriguing quantum properties that are unique for 1D system.

EMILY L. QUE, F-1883, The University of Texas at Austin. EXPLORING THE USE OF Cu(II) IN ¹⁹F MAGNETIC RESONANCE CONTRAST AGENTS FOR IMAGING BIOLOGICAL REDOX.

In this grant year, our research in contrast agent development focused on: A) developing fluorine dense and nanoparticulate systems for ¹⁹F MR-based biosensing, including Cu-based hypoxia sensing nanoemulsions B) developing Ni-based scaffolds for pH sensing and C) developing targeted imaging agents for metalloenzymes.

A) One major limitation of ¹⁹F MRI is lack of signal intensity. We have submitted one manuscript for Co- based sensing of oxidative activity based on a highly fluorinated scaffold. In our efforts to implement ¹⁹F probes in vivo, we are expanding our probe systems to include fluorine-rich nanoparticles that can be used as bioresponsive imaging agents. These include stable nanoemulsions based on combinations of highly fluorinated Cu-hypoxia sensors and biocompatible oils. We have completed in vitro testing of nanoemulsion agents and now have an approved animal protocol to implement them in in vivo hypoxia models.

B) In addition to redox-activated imaging agents based off of Cu(II) and Co(II), Ni(II) scaffolds can be exploited for sensing based on the fact that square planar Ni(II) is diamagnetic and octahedral Ni(II) is paramagnetic. We are exploring sterically hindered macrocycles with pendant bases as scaffolds for pH sensing, where the pendant base is bound to the Ni at basic pH values (giving a paramagnetic signal) and becomes protonated at acidic pH values, yielding a diamagnetic Ni center. We have submitted a proof- of-concept system for publication.

C) Finally, looking to the future, we would like to use ¹⁹F imaging agents for detecting proteins in vivo, looking towards imaging proteins of interest to cancer. Towards this goal, we have published a proof-of- concept paper (Chem Commun 2018) demonstrating the use of a small molecule probe for imaging carbonic anhydrase (a hypoxia-relevant protein) in cells and currently are expanding this area to include ¹⁹F agents and other probe types.

ARUN RADHAKRISHNAN, I-1793, The University of Texas Southwestern Medical Center. MOLECULAR MECHANISMS OF CHOLESTEROL SENSORS IN HUMAN CELLS.

In the past year, we have made progress towards obtaining a high-resolution structure of Scap, a polytopic cholesterol-sensing membrane protein that allows cells to maintain an optimal concentration of cholesterol. We have solved several technical hurdles to obtain milligram quantities of recombinant Scap locked in its cholesterol-bound conformation. We have also obtained milligram quantities of Insig, an endoplasmic reticulum-resident membrane protein that forms complexes with Scap when cholesterol levels are high, and have reconstituted the Scap/Insig complex in vitro.

We are currently pursuing a combination of crystallographic and cryo-electron microscopy approaches to obtain the first structures of Scap and Scap/Insig complexes.

Additionally, we were invited by the Annual Review of Biochemistry to prepare a review article on Scap. This comprehensive review chronicling the discovery, cell biological characterization, and molecular mechanistic studies of Scap was published in 2018.

MARK G. RAIZEN, F-1258, The University of Texas at Austin. IMAGING OF SURFACE CHEMISTRY WITH NEUTRAL ATOMS.

We implemented a technique to brighten the atomic beam before it reaches the pulsed hexapole lens. The beam is focused by a permanent magnetic hexapole made with rare earth magnets. At the permanent lens's focal point we collimate the beam by performing laser cooling in two directions transverse to the beam's velocity. The combination of these techniques decreased the beam width by a factor of 3.7 and increased the beam density by a factor of 20.

We also implemented the pulsed magnetic hexapole lens further downstream, which again increased the peak density of the atomic beam by factor of 20. This does not necessarily imply a total increase by a factor of 400, because the data for the two lenses were taken at different points along the beamline. We also demonstrated the tunability of this lens by changing its focal length by altering the current that passes through the lens.

We are addressing two technical limitations which have prevented us from seeing the full benefits of the pulsed lens. First, we used a pulse length that is longer than the time required for the atoms to pass through the lens, so the lens was effectively operating in a DC mode. To address this issue we have modified our electronic circuits to achieve shorter pulses. Second, the resolution of our detection system prevents us from measuring beam widths smaller than 150 μm . We have installed a new detection system which sweeps a knife-edge across the beam. By measuring the resulting change in flux we can measure beam width on a nanometer scale.

RAMA RANGANATHAN, I-1366, The University of Texas Southwestern Medical Center. EVOLUTIONARY DYNAMICS AND THE DESIGN OF NATURAL PORTEINS.

Over the last year we have continued our studies on protein design and evolution. As mentioned briefly in the last progress report, our study describing a new method to determine the internal mechanics of proteins was published (Nature 2016, 540: 400-405). We showed that the application of electric field pulses to protein crystals drove concerted motions within proteins that could be mapped by time-resolved X-ray crystallography. In turn, the tracked motions provided new insight into local and allosteric conformational changes within the protein that were required for function. Going forward, the application of our method should prove useful in elucidating the mechanical bases of protein function. In a second published study (eLife 2017, doi: 10.7554/eLife.27810), we continued our analysis of the mutational tolerance of proteins, focusing on Ras, an oncogene activated in lung and other cancers. Saturation mutagenesis was used to create a library of altered Ras proteins in which the amino acid sequence was randomized one position at a time. By analyzing each mutant protein using a two-hybrid assay, we found that mutational tolerance was low in regions bound by interacting proteins such as activators

and suppressors of Ras. These data indicate that mammalian Ras is co-evolving with its regulators and that the overall sequence conservation observed in Ras proteins from different species arises largely from the biochemical network in which the protein must act.

This will be the last progress report associated with this grant; I have taken a faculty position at the University of Chicago where I will continue my research on protein dynamics.

FRANK M. RAUSHEL, A-0840, Texas A&M University. ELUCIDATION OF ENZYME REACTION MECHANISMS.

Sphingobium sp. SYK-6 is a Gram-negative soil bacterium that contributes to the degradation of lignin. Lignin provides structural support and protection to plants as a complex aromatic heteropolymer. The lignin degradation pathway of guaiacyl moieties leads to the intermediate, protocatechuate (PCA), which is further degraded via the 4,5-cleavage pathway where PCA is ultimately metabolized to pyruvate and oxaloacetate. In this pathway, LigI has been shown to catalyze the hydrolysis of 2-pyrone-4,6- dicarboxylate (PDC) to (4E)-oxalomesaconate (OMA). We have demonstrated, using ¹H and ¹³C NMR spectroscopy, that LigU catalyzes the isomerization of the double bond between C4 and C5 in (4E)-OMA to (3Z)-2-keto-4-carboxy-3-hexenedioate (KCH), where the double bond has migrated to be between C3 and C4 via a 1,3-allylic isomerization. LigU is most closely related in amino acid sequence to methylaconitate isomerase (PrpF) from *Shewanella oneidensis* and methylitaconate- isomerase (Mii) from *Eubacterium barkeri*. The kinetic constants for the isomerization of OMA to KCH by LigU at pH 8.0 were determined to be 1300 ± 120 s⁻¹ and $7.7 (+ 1.5) \times 10^6$ M⁻¹ s⁻¹ for *k*_{cat} and *k*_{cat}/*K*_m, respectively. We have shown that the product of the LigU catalyzed reaction is the preferred substrate for the LigJ hydratase. In this reaction LigJ catalyzes the hydration of KCH to 4-carboxy-4- hydroxy-2-oxoadipate (CHA).

JOSEPH M. READY, I-1612, The University of Texas Southwestern Medical Center. NEW DIRECTIONS IN ASYMMETRIC SYNTHESIS.

In our first aim, we have been expanding the scope of the 3-component coupling. We have now shown that the reaction can be used to establish adjacent quaternary stereocenters, which remain challenging substructures to access, especially in optically active form. Thus, indoles featuring a substituent at the C3 position can be lithiated at C2, combined with an alkyl or aryl boronic ester, and allylated in the presence of a Pd-catalyst. The products feature an allyl/alkyl quaternary center at C3 of the indole and an alkyl/boron or aryl/boron quaternary stereocenter at C2. In this work, we made several significant discoveries. First, we identified a class of phosphorus ligands that had not previously been used with Pd. Mechanistic studies support the intermediacy of a mono-dentate, mono-ligated P*Pd(allyl)OAc complex as the reactive intermediate. Second, products were formed with high yields, enantioselectivities and diastereoselectivity. Stereochemical probes indicated a stepwise process for the reaction, which was in contrast to literature proposals for related transformations.

In the second aim of the proposal, we have derivatized the C-B bond by converting it to C-H, C-O, and C-C bonds. First, we found that protodeborylation proceeded with retention of stereochemistry to provide indolines with high *er* and *dr*. Second, oxidation of the allyl group (Wacker or hydroboration/oxidation) and cyclization onto the C2 position formed fused tetrahydrofurans or tetrahydropyrans. Finally, several photochemical transformations were identified. For example, irradiation of the boronic esters in the presence of a Michael acceptor (cyanoacrylate, methyl acrylate) results in a 1,4-addition. Surprisingly for a radical process, the reaction is highly diastereoselective. When methyl- vinyl ketone is the acceptor, an unexpected annulation occurs which involves 1,4-addition, 1,5-hydrogen abstraction, and addition to a ketone. Mechanistic studies are ongoing to understand this process.

MICHAEL REESE, I-1936, The University of Texas Southwestern Medical Center. UNRAVELLING THE NON-CANONICAL ACTIVATION MECHANISM OF TOXOPLASMA KINASES.

This Welch Fellowship funds research on Toxoplasma kinases through my postdoctoral fellow Dr. Xiaoyu Hu. Dr. Hu has successfully completed significant aims in her project, and we expect to begin work on at least one manuscript by the end of the calendar year. Specifically, working with other members of my team, Dr. Hu has determined that TgMAPKL2 is essential for replication of the parasite and appears to license the cellular machinery required for parasite budding. We have also demonstrated that a second TgMAPK, TgERK7, appears to be essential for secretion of molecules that the parasite requires to move and invade host cells. We hope to complete a manuscript detailing this finding in the next year.

LINDA E. REICHL, F-1051, The University of Texas at Austin. RELAXATION PROCESSES IN ULTRACOLD ATOMIC MIXTURES AND DISSOCIATED MOLECULES.

(1) Open quantum systems can serve as models for small molecules, nanoscale quantum devices, and electromagnetic wave dynamics in optical micro cavities.

We have shown that Wigner-Eisenbud scattering theory can be used to analyze the transmission probabilities, delay times, and quasibound state structures in 2D and 3D open quantum systems. To test the method, we considered an open quantum system consisting of three Gaussian potential energy peaks, sitting in the continuum. This is a system whose classical dynamics is known to be chaotic. We determined energy regimes with the quantum manifestations of chaos. We derived an exact expression for the non-Hermitian Hamiltonian whose eigenvalues give the complex quasibound state energies and the delay times of these long-lived quantum states in the continuum.

(2) We also developed another very promising use of Wigner-Eisenbud scattering theory. We have used it to analyze decay processes in the neighborhood of a periodic lattice. We found that the decay processes can be described in terms Bloch momentum channels. For the case where the periodic lattice has reflection symmetry, we found that the lattice can sustain bound states in the continuum. These are states in the continuum that have infinite lifetime. They are prevented from decaying by the underlying spatial symmetry of the lattice.

(3) We are expanding our work on Bose-Einstein condensates to now include superconductors. We obtained exact expressions for the current and shot noise in an NSN (normal-superconducting-normal) nanowire. These expressions involve inelastic scattering processes and are a function of the superconducting gap, the Fermi energies, effective masses, and the temperature. We found that, unlike low-Tc superconductors, several high-Tc cuprate superconductors can sustain current flow in nanowires with width as small as the coherence length of the superconductor.

PENGYU REN, F-1691, The University of Texas at Austin. MULTISCALE MODELING OF RNA 3D STRUCTURE AND FOLDING.

Previously we have developed a preliminary coarse-grained (CG) RNA model, named RACER (RnA CoarsE-gRained). The RACER model has been successfully applied to fold small RNA motifs including helices, hairpins, and co-axial stacking with CG molecular dynamics and to perform pulling free energy simulations. This past year we have been focusing on the noncanonical hydrogen bonding in RNA base pairs, which are crucial for the structure and stability large RNA structures beyond duplexes and hairpins. We have sampled a wide range of RNA base pairing configurations from Protein Data Bank, and utilized quantum mechanical calculations to characterize the strength of base pairing in "implicit" solvent. Based on these data, we have systematically parameterized and incorporated non-canonical hydrogen-bonding potential into the RACER model. Initial pulling simulations have demonstrated that RACER model captures the thermodynamic stability of G-quadruplexes and the enhancing effect of K⁺ ions. Meanwhile, we have also made significant progress on atomistic polarizable nucleic acid force fields which will be coupled with the CG model in the future for multi-scale investigation of RNAs.

PETER M. RENTZEPIS, A-1884, Texas A&M University. TIME AND SPACE RESOLVED CHEMICAL AND BIOLOGICAL REACTION INTERMEDIATES.

During the past year, with partial Welch foundation support, we have performed several experimental studies using our novel a new femtosecond we have studied with fs and Angstrom resolution the atomic rearrangement mechanism of melting recrystallization and lattice deformation in polycrystalline Al and Al (111) single crystals. These studies have resulted ... publications, one international patent and three invited talks. In May 2018 two students, received their BS with high honors and one was awarded the MS degree. At the present time two undergraduate, two graduate students and a postdoctoral scientist are pursuing research, in our labs with partial support by The Welch Foundation grant.

II. Ultrafast structural dynamics. The experimental femtosecond electron and x-ray system was described previously, (1), It made it possible to determine the dynamics of lattice expansion, contraction, heat propagation, atomic melting and recrystallization with fs time and Angstrom resolution Al (111) and Al polycrystalline.

We measured the heat distribution from the initial pumping to an electron temperature of 104 K on the surface of the crystal within 7 ps to a temperature of 300 K within the bulk of Al (111) crystal after 120 ps, Using the two-Temperature Model we simulated the effect of pumping a 150 nm thick Al (111) crystal with a 18.5 mJ/cm² femtosecond laser pulse. By these calculations we determined the spatial- temporal distribution of the electron temperature and calculate the spatial-temporal distribution from the lattice temperature of the surface to its propagation through the bulk as a function of time

Another area of research concerns the detection, identification of bacteria in situ within a few minutes and the determination of the live: dead bacteria ratio, in remote areas as a function of reaction time against antibiotics. The bacteria studied were .coli and bacillus reacting against several antibiotic drubs including polymixin B and ampicilli.

LUKE M. RICE, I-1908, The University of Texas Southwestern Medical Center. STRUCTURE AND BIOCHEMISTRY OF A MICROTUBULE REGULATORY PROTEIN.

The research supported by this award is primarily focused on the linker-TOG2 fragment from the microtubule regulatory factor Stu1. Stu1 is a member of the evolutionarily conserved CLASP family of proteins. CLASPs promote microtubule rescue, the switch from shrinking (depolymerization) back to growing (polymerization). The molecular mechanism of CLASP activity is not known, but is thought to require coordinated action of multiple TOG domains. During this granting period, we published a paper that contradicted this expectation that coordinated action of multiple TOGs would be required for rescue activity. Our paper showed that the isolated linker-TOG2 fragment could potently stimulate rescue and that is also suppressed catastrophe (the switch from microtubule growing to microtubule shrinking). The linker-TOG2 fragment regulated these transition frequencies without affecting microtubule growing or shrinking rates, and we identified a previously unknown, CLASP-specific conserved residue that through our structural analysis.

Although linker-TOG2 can by itself stimulate rescue and suppress catastrophe, it is clear that other regions of the protein contribute to this activity. During the last granting period, we showed that the larger, TOG1-linker-TOG2 fragment of Stu1 was more potent than linker-TOG2, even though the isolated TOG1 domain does not appear to interact appreciably with ab-tubulin. Discovering the basis for this enhanced activity will be a focus of the next granting period, as will obtaining structures for linker-TOG2 or TOG1-linker-TOG2 bound to ab-tubulin or microtubules.

Finally, in studies of the TOG-domain-containing microtubule regulatory factor Stu2, which acts to enhance microtubule growth rates, we published a paper demonstrating how its activity depends on the number of TOG domain and proposing a model for the molecular mechanism of its processive action.

MICHAEL G. RICHMOND, B-1093, University of North Texas. SYNTHESIS AND REACTIVITY STUDIES OF POLYNUCLEAR CLUSTERS.

The site preference for ligand substitution in the benzothiazolate-bridged cluster HO₃(CO)₁₀(u-1,2- N,C-n1,n1-C7H4NS) (1) has been investigated using PPh₃. Cluster 1 reacts with PPh₃ in the presence of Me₃NO to afford the mono- and bisphosphine substituted clusters HO₃(CO)₉(PPh₃)(u-

1,2-N,C- n1,n1-C7H4NS) (2) and $\text{HOs}3(\text{CO})8(\text{PPh}3)2(\text{u-1,2-N,C-n1,n1-C7H4NS})$ (3), respectively. Cluster 2 has been shown to exist as a pair of non-interconverting isomers where the $\text{PPh}3$ ligand is situated at one of the equatorial sites syn to the edge-bridging hydride that shares a common Os-Os bond with the metalated heterocycle. The solid-state structure of the major isomer establishes the $\text{PPh}3$ regiochemistry at the N-substituted osmium center. Electronic structure calculations have confirmed the thermodynamic preference for this particular isomer relative to the minor isomer whose phosphine ligand is located at the adjacent C-metalated osmium center. Control experiments reveal that cluster 2 reacts with $\text{PPh}3$ to give 3. The locus of the second substitution occurs at one of the two equatorial sites at the $\text{Os}(\text{CO})4$ moiety in 2 and gives rise to a pair of fluxional stereoisomers where the new phosphine ligand is scrambled between the two equatorial sites at the $\text{Os}(\text{CO})3\text{P}$ moiety. The molecular structure of the major isomer has been determined by X-ray diffraction analysis and found to represent the lowest energy structure of the different stereoisomers computed for $\text{HOs}3(\text{CO})8(\text{PPh}3)2(\text{u-1,2-N,C-n1,n1-C7H4NS})$. The fluxional behavior displayed by 3 has been examined by VT NMR spectroscopy, and DFT calculations provide evidence for stereoselective tripodal rotation at the $\text{Os}(\text{CO})3\text{P}$ moiety that serves to equilibrate the second phosphine between the two available equatorial sites. The separation of these new chiral clusters has been explored and their chiral-optical properties probed during this funding period.

JEFFREY D. RIMER, E-1794, University of Houston. PHYSICOCHEMICAL FACTORS GOVERNING PROTEIN INHIBITION OF CALCIUM OXALATE MONOHYDRATE CRYSTALLIZATION.

The past year of this project supported three graduate students and resulted in 11 published articles, 3 accepted articles, and 2 submitted manuscripts. Research on calcium oxalate monohydrate (COM) crystallization has primarily focused on the identification of small organic acids that were found to exhibit unique modes of growth inhibition. We have expanded the study of hydroxycitrate, which is a putative drug for human kidney stones. We also discovered that phosphate molecules are potent inhibitors of COM nucleation. We are now investigating the potential use of cooperative modifiers of COM crystallization (carboxylates and phosphates) as a platform for combination therapies. As part of this Welch project, we have developed a new technique for rapidly screening crystal growth using microfluidic devices to more efficiently conduct parametric studies and identify new pathways to tailor the physicochemical properties of crystals. To this end, we have expanded our study of human kidney stone minerals to brushite and struvite. We have also extended this line of research to studies of beta-hematin crystallization, which is a byproduct heme detoxification in malaria. During the past year we identified the modes of action for several common antimalarial drugs (crystal growth inhibitors), which we published in PNAS. We have also discovered the mechanism by which artemisinin functions as a crystal growth inhibitor. Another major breakthrough in this project was the design of a liquid AFM cell for solvothermal imaging, which we used to explore the growth microporous materials (e.g. zeolite A) and observed new crystallization pathways that have never been reported in literature. This work was published in Nature Communications and has spurred continued investigation of complex mechanisms of nonclassical zeolite crystallization. Collectively, these projects are part of a broader initiative to elucidate crystallization pathways and develop materials through rational design.

JOSE RIZO-REY, I-1304, The University of Texas Southwestern Medical Center. NMR METHODS TO STUDY MEMBRANE PROTEINS IN LIPID BILAYERS.

We completed a study of how complexin interacts with the neuronal SNARE complex formed by syntaxin, synaptobrevin and SNAP-25, which mediates synaptic vesicle exocytosis (Prinslow et al., 2017). These interactions were known to be critical to regulate neurotransmitter release, but there was a controversy as to how the accessory helix of complexin inhibits release. Using isothermal titration calorimetry, we showed that the accessory helix does not interact with the SNARE complex, in agreement with nuclear magnetic resonance (NMR) data and with a model whereby the accessory helix hinders membrane fusion due to steric hindrance with the membranes. However, we observed an interaction of the complexin N-terminal region with the juxtamembrane region of syntaxin, which explains the controversy that had arisen. In separate work (Voleti et al., 2017), we investigated the basis for the distinct functional importance of Ca^{2+} binding to the two C2 domains of synaptotagmin-1 and synaptotagmin-7, which act as Ca^{2+} sensors for synchronous and asynchronous neurotransmitter release, respectively. We determined the crystal structures of fragments spanning the C2 domains of synaptotagmin-7, which were very similar to those of synaptotagmin-1 C2 domains. However, we found that the synaptotagmin-7 C2A domain plays a predominant role in membrane binding, whereas such predominant role is played by the C2B domain in synaptotagmin-1, in agreement with the relative functional importance of these domains in the respective isoforms. In another study (deJong et al., 2018), we showed that the RIM C2B domain binds to PIP2 using NMR and demonstrated the critical importance of this interaction for neurotransmitter release. We also published a detailed protocol for the reconstitution of basic features of synaptic vesicle fusion with the eight most central proteins of the neurotransmitter release machinery (Liu et al., 2017), and a review of our research in this area (Rizo 2018).

SEAN T. ROBERTS, F-1885, The University of Texas at Austin. MAPPING SINGLET EXCITON FISSION AND ENERGY TRANSPORT PATHWAYS IN PERYLENE DIIMIDE THIN FILMS AND CRYSTALS WITH FEMTOSECOND TIME-RESOLVED SPECTROSCOPY.

We have investigated factors that dictate the singlet fission (SF) rate in perylenediimide (PDI) solids, whose structure we can control via functional groups placed at the PDI imide position. We find SF rates for different PDI packing arrangements are in good agreement with structural trends predicted by Redfield theory. However, the magnitude of the measured rates are $\sim 1000\times$ slower than theory predictions. Using a site-based Hamiltonian to calculate state energies involved in SF, we have traced this discrepancy to a ~ 200 meV activation barrier for SF that is overlooked in the Redfield treatment. This work appeared in J. Am. Chem. Soc. in January. We have since shifted our focus to designing semiconductor interfaces to extract spin-triplet excitons produced by SF. As a model, we have studied PbS nanocrystals functionalized with SF-capable acene molecules as this system eliminates issues tied to exciton diffusion to the acene:semiconductor interface. We find spin-triplet excitons can readily transfer from one material to the other, but do so via a long-lived intermediate state

that spans their interface. A report describing our findings was published in J. Am. Chem. Soc. in May. We are now investigating PDI films grown on Si(111) surfaces terminated with either hydrogen or methyl capping groups. We observe strong photoluminescence quenching for PDI films on Si(111) and find PDI excited state kinetics are strongly altered by the presence of Si. We are currently using electronic sum frequency generation to examine the electronic structure of the PDI:Si junction. Preliminary data suggests strain-induced changes in PDI packing structure at the Si surface lower PDI spin-singlet and spin-triplet exciton energies, creating an energetic funnel that can direct excitations to the Si interface and aid energy extraction. Over the past year, Welch Foundation support was acknowledged in 10 oral presentations by the PI and 5 oral/poster presentations by graduate students.

DANIEL ROMO, A-1280, Texas A&M University. NOVEL STRATEGIES FOR β -LACTONE SYNTHESIS AND ANNULATION TO IMPACT BASIC CELL BIOLOGY.

We are continuing to optimize the flow reactor version of the allylic bromination, zinc reagent formation, CO₂ capture, bromo-lactonization sequence developed previously making use of higher concentrations of dissolved CO₂ enabled through tube-in-tube reactors. Beta-Lactones and beta-lactams were previously introduced into andrographolide and yohimbic acid and more recently a beta-lactone was annulated onto perillyl alcohol and a beta-lactam was annulated onto caryophyllene oxide, alpha-pinene, aromadendrene, and isopropenyl adamantane. All these derivatives have or will be tested against pathogenic bacteria and various cancer cell lines (collaborator: Prof. Stephan Sieber, TU München, Germany). Our function-oriented synthesis of the anticancer agent, hypercalin C, enabled a brief SAR profile in collaboration with Asst. Prof. Joe Taube (Baylor Univ.) and a manuscript on this work will be submitted soon.

MICHAEL J. ROSE, F-1822, The University of Texas at Austin. EARTH ABUNDANT METAL CATALYSTS FOR ENERGY-RELATED CHEMICAL TRANSFORMATIONS.

In the past year we have made significant progress along three avenues:

(1) Iron-based H₂ catalysts: We have continued to develop our anthracene-based scaffold ligand strategy to replicate the reactivity of a hydride transfer enzyme, mono-iron hydrogenase. Most notably, based on the novel incorporation of a thiolato-S donor, we have replicated the hydride transfer reactivity of the enzyme in a small-molecule format. Our 2018 *Angew Chem* paper (denoted a VIP paper) demonstrates sequential H₂ activation and hydride transfer. The role of this thiolato-S donor in stabilizing or thermalizing CO ligands was explored in a related *Inorg Chem* paper, wherein we demonstrated that the sulfur donor, itself, is not sufficient to impart thermal stability to the dicarbonyliron core of the active site. This highlights the critical need for the organometallic Fe-C bonding motif in our other functional model compounds. We also published a review that outlines the overall precedents, rationale and approach for using anthracene-like scaffolds in bio-inorganic chemistry and catalysis.

(2) We have successfully incorporated a molybdenum atom into a carbide-based cluster as a structural relative of the nitrogenase active site cluster. This heterometallic Fe/Mo-containing cluster (denoted Fe₅Mo) selectively reduces E-E triple bonds, transforming diphenylacetylene into cis-diphenylethylene.

(3) Lastly, in the silicon-surface / solar energy project, we demonstrated a rational approach to modifying silicon semiconductor (solar cells) with organic moieties of varying steric sizes. This has laid the critical framework for assembling a hybrid molecular materials solar conversion device, using sterically spaced molecular wires (embedded in a metal oxide matrix) as electron transfer mediators. Such work is presently ongoing.

MICHAEL K. ROSEN, I-1544, The University of Texas Southwestern Medical Center. 2D PHASE SEPARATED PROTEIN POLYMERS: INTERACTIONS WITH ACTIN FILAMENTS.

In Aim 1 we have tested our hypothesis that membrane dwell time controls the activity of N-WASP in two ways. First, we analyzed dwell time of N-WASP: inside vs outside of clusters formed with membrane-attached Nephhrin; in clusters formed by Nck analogs containing 6 or 3 SH3 domains; bound to membrane-associated Nck in the presence or absence of clustering by soluble Nephhrin. In all cases, longer membrane dwell time corresponded to higher activity toward the Arp2/3 complex. Second, we ran a series of titrations where Nephhrin and N-WASP were fixed, and Nck concentration was varied. As predicted by computational modeling of connectivity in the network, the dwell time of N-WASP was short at low and high Nck, and peaked for intermediate levels. Correspondingly, actin assembly activity was low at the extremes of Nck and highest in the middle regime. We also used single-molecule imaging to demonstrate that the lifetime of the Arp2/3 complex paralleled that of N-WASP. This result demonstrates two general principles. First, for phase separated transmembrane signaling pathways with appropriate characteristics, dwell time of intracellular components should control activity. Second, variations in stoichiometry represent a new, general mechanism to control protein specific activity, which is unique to stoichiometrically undefined systems, such as phase separated clusters. In Aim 2, we have examined a battery of Nck and N-WASP deletion mutants, and found that basic regions of both proteins mediate adhesion to actin filaments. Moreover, when the N-WASP basic region is attached to the Grb2 protein in Jurkat T cells, creating aberrantly strong adhesion between Grb2-LAT clusters and actin filaments, the clusters move improperly at the surface of an activated T cell. This work has led us to a model that explains how LAT clusters move radially in activated T cells through two distinct actin networks, which require different levels of cluster-actin adhesion.

DANIEL M. ROSENBAUM, I-1770, The University of Texas Southwestern Medical Center. CAPTURING THE ACTIVE CONFORMATIONS OF CNS GPCRS WITH NANOBODIES.

Over the past year of Welch Foundation support, my lab has made significant progress in our biophysical studies of physiologically important CNS GPCRs. We primarily work on the orexin and CB1 cannabinoid receptors, GPCRs regulating circadian rhythms and synaptic homeostasis and therapeutic targets for multiple diseases. We recently solved the high-resolution structure of CB1 bound to a high-affinity synthetic agonist, which will aid in the

structure-guided drug design of novel CB1 modulators. We also collaborated to report the structure of OX2R bound to a type 2 selective inhibitor, so that we now have high-resolution models for antagonist selectivity in both orexin GPCRs. For each of these GPCRs, we have sent purified samples to a collaborator (Jan Steyaert in Belgium) to raise nanobodies in-vivo.

Characterizing the resulting nanobodies is still in progress, however we have had difficulties with a high rate of non-specific clones. As a result, we have implemented a fully in-vitro nanobody selection by yeast display, in which we can completely control the nature of the antigen. We plan to characterize our first nanobodies arising from these in-vitro selections in the coming months. Meanwhile, we have made a significant breakthrough in the development of NMR labeling techniques that allow incorporation of magnetically active isotopes into purified GPCRs. This system allows us to probe GPCR structure and dynamics on multiple timescales. We published our first paper using this method to characterize a GPCR in October 2017 in eLife, and we have been making progress extending the method to other GPCRs including the orexin receptors and CB1. In the coming year, we anticipate purifying our first GPCR/nanobody complexes, and we hope to obtain our first diffraction quality crystals on these complexes. Further, we plan to use our GPCR NMR platform to look for specific patterns of dynamic structural change that are unique to the neuropeptide and lipid GPCR families.

JOSEPH H. ROSS, JR., A-1526, Texas A&M University. **MAGNETIC, ELECTRONIC AND DYNAMICAL BEHAVIOR OF NEW SEMICONDUCTING MATERIALS.**

This year our work included new measurements of Cu₁₂Sb₄S₁₃-based tetrahedrites, which are of interest as thermoelectrics, with strongly anharmonic vibrational modes contributing to a very low thermal conductivity. By assessing the Cu quadrupole-NMR T₁, we identified a large relaxation-rate response providing a quantitative measure of Cu-ion displacements as complement to crystallographic measurements, both above and below the metal-insulator transformation in un-substituted Cu₁₂Sb₄S₁₃. In addition, from changes in the NMR line-shapes we identified a set of atomic distortions occurring above this transformation, for which details have remained uncertain. In further measurements of Zn and Ni-substituted compositions we demonstrated changes in the anharmonic vibrational mode, which remains despite the atomic disorder and complete suppression of the structural transformation by metal-ion substitution. This is important since metal substitution tunes the behavior for thermoelectric applications, but makes standard crystallographic assessment difficult. Additional work focused on half-Heusler semiconductors, including native and Ti-substituted NbFeSb, also of significant recent interest as practical thermoelectric materials. In a series of measurements including a detailed NMR study, we focused on the native defects which dominate the electronic and thermal transport. We demonstrated a new method which can be used to separate paramagnetic contributions to the NMR T₁ relaxation, and together with specific heat and magnetization measurements identified a native defect dominating the magnetic behavior of p-type NbFeSb. This further allowed us to probe the underlying charge carrier behavior, which we found to be connected to an impurity band due to an additional set of native defects. We also initiated measurements of several other materials, including NMR studies of ScPt_xPd_{1-x}Bi, which features a topological band inversion in its crossing to a semimetallic behavior.

PETER ROSSKY, C-1937, Rice University. **UNDERSTANDING CONJUGATED POLYMER AGGREGATION AND OPTOELECTRONIC PROPERTIES VIA MULTISCALE SIMULATION.**

We have made excellent progress implementing the computational tools needed to span the full spectrum of scales for both spatial and electronic structures.

Specifically, we have:

Substantially improved our coarse-grain model for the semi-conducting polymer P3HT. A recently published all-atom molecular mechanics potential claimed to describe polymer energy dependence on polymer twisting (dihedral) angles was found not to be accurate compared to our well-tested semiempirical quantum chemistry approach. We repeated our Bayesian optimization of our coarse-grain model to reproduce the statistical structures obtained directly from our quantum model.

Demonstrated unique capacity of our model to calculate electronic structure from coarse-grain structures. This is enabled by the demonstration of an accurate reverse mapping of the coarse-grain structure to an all-atom structure, a unique feature of our model.

Explored the use of implicit and explicit solvation models. By comparison of all-atom and coarse grain model behavior, we have established satisfactory performance of a coarse grain model for an appropriate solvent (chlorobenzene).

Studied emergence of order upon formation of conjugated polymer assemblies. By studying a series of well-defined multi-chain aggregates, we have developed appropriate metrics that can identify regions having characteristic backbone order analogous to liquid crystals and regions having sequential correlation of backbone twists (particularly planarity).

Explored machine learning algorithms to identify spatial structures having target electronic properties. Using a training set of structures generated with simulation of the coarse-grain model and electronic excitation energies calculated from reverse mapping of structures, we find very encouraging results for sets of correlated dihedral angles that map to a target excitation energy.

RICK RUSSELL, F-1563, The University of Texas at Austin. **INVESTIGATION OF RNA MISFOLDING ALTERED TOPOLOGY.**

We made substantial progress in the past year on several fronts. First, our understanding of the mechanisms through which DEAD-box helicases remodel RNAs was advanced, and we were able to contrast these mechanisms explicitly with those of the related DEAH-box helicases. This work was published in the journal Biochemical Society Transactions. Second, we turned our attention to a new class of RNA and DNA structure, the widespread G-quadruplex (G4), and a DEAH-box helicase that interacts specifically with G4s and disrupts them. We elucidated the mechanism of this disruption as a

conventional DEAH-box mechanism and published this work in the Journal of Biological Chemistry. This work also showed that DHX36 is highly specific for disrupting G4s and that binding is rate-limiting for G4 disruption under standard conditions, underscoring the efficiency of this enzyme. Our work suggests that DHX36 is a dominant force mediating G4 disruption in vivo. Third, we continued a dissection of DEAD-box helicases by asking whether the helicase core and ancillary 'C-tail' of the DEAD-box protein CYT-19 function as independent modules. Our results showed that they indeed give energetically independent effects on RNA binding and that appending an exogenous RNA-binding element in place of the C-tail changes the RNA-binding specificity of CYT-19 in a predictable way without modulating the properties of the helicase core. This work in preparation for submission within the next two to three months.

LIVIA SCHIAVINATO EBERLIN, F-1895, The University of Texas at Austin. DEVELOPMENT OF AMBIENT IONIZATION ION MOBILITY MASS SPECTROMETRY IMAGING FOR SPATIAL AND CHEMICAL LIPID ANALYSIS IN BIOLOGICAL SAMPLES.

During Year 2 of Welch Grant, we explored integration of desorption electrospray ionization mass spectrometry (DESI-MS) to a high-field asymmetric waveform ion mobility spectrometry (FAIMS) device for imaging proteins from biological tissue sections. Analysis of large biomolecules including proteins has proven challenging using ambient ionization mass spectrometry imaging techniques. Within the last year, we successfully optimized DESI-MS experimental parameters to detect intact proteins directly from tissue sections. In an effort to further increase S/N of proteins, we integrated FAIMS to the DESI-MS imaging source and mass spectrometer interface as we have previously described. Two-dimensional FAIMS sweep experiments were performed to determine the optimal dispersion field ($DF = 180$ Td) and compensation field ($CF = +1.0$ Td) for protein detection. Under the optimized FAIMS parameters, improved S/N was achieved for alpha-globin proteoform, as well as detection of 10 other distinct protein species. The addition of FAIMS increased the S/N for all the proteins detected due to the substantial filtering of interfering background species (68% decrease), including abundant solvent peaks, and reduction of chemical noise (43% decrease), despite an overall drop (30%) in the absolute intensities of protein ions. Optimized DESI-FAIMS-MS parameters were used to image mouse kidney, mouse brain, and human ovarian and breast tissue samples, allowing detection of 11, 16, 14, and 16 proteoforms, respectively. Protein identification was performed on-tissue by top-down ultraviolet photodissociation (UVPD) and collision induced dissociation (CID). Our results demonstrate that DESI-MS imaging is suitable for the analysis of the distribution of proteins within biological tissue sections. In year 3, we plan to continue to explore FAIMS integrated to DESI imaging to investigate the distribution.

SANDRA L. SCHMID, I-1823, The University of Texas Southwestern Medical Center. DISSECTING DYNAMIN ISOFORM-SPECIFIC REGULATION OF CLATHRIN MEDIATED ENDOCYTOSIS.

Aim 1: All constructs have been prepared and assays are in place. A new postdoctoral fellow, Madhura Bhawe is now partially supported by this grant and embarking on these experiments.

Aim 2: Zhiming Chen, another new postdoc supported by the Welch has completed 3 rounds of pulldown and proteomic experiments comparing the interactomes of GST-Dyn1-PRDWT, GST-Dyn1-PRDAA, GST-Dyn1-PRDEE and GST-Dyn2PRDWT. Interestingly, SNX9 and actin regulators preferentially bind to Dyn1-PRDAA over Dyn2. The function significance of SNX9 binding was validated and published in Srinivasan et al., 2018. The significance of Dyn1 specific actin interactions are being investigated.

Aim 3: We have completed this aim and a paper describing our findings was published in PLoS Biology (Srinivasan et al., 2018). Briefly, we found that Dyn1 and Dyn2 are recruited to the same CCPs, although to varying extents. Even when barely detectable on CCPs' Dyn1 activation downstream of GSK3 inhibition accelerates CCP initiation and maturation rates. SNX9 is selectively required for the Dyn1 effects on CCP maturation. Dr. Srinivasan has left the lab for a research position at Pfizer in St.

Louis.

We also accepted an invitation to write a comprehensive review for the prestigious Annual Review of Biochemistry on the regulation of clathrin-mediated endocytosis, which included discussion of our identification of dynamin as a major regulator of early events in CME.

HANS A. SCHUESSLER, A-1546, Texas A&M University. OPTICAL STUDIES OF ATOMIC AND MOLECULAR SYSTEMS WITH FEMTOSECOND, XUV AND IR LASER RADIATION.

A single comb line of an optical frequency comb was used to excite target transitions of a single ^{25}Mg ion confined in a Paul trap to realize direct frequency comb spectroscopy and measurements of the absolute transition frequencies. We demonstrated that direct frequency comb spectroscopy can extend optical frequency metrology into the deep UV spectral regions unreachable by continuous wave lasers. The formation of positively charged fragments of acetonitrile (CH_3CN) and ethane in intense 800 nm, 50 fs pulses of radiation was investigated using a reflectron time-of-flight (TOF) ion mass spectrometer. For angular dependences of yields of ions C^+ , C_2^+ and C_2H_2^+ besides maxima for parallel polarizations also maxima in perpendicular directions were observed. Kinetic energies of hydrogen fragments H^+ , H_2^+ and H_3^+ were experimentally measured. For trace methane detection in ambient air we employed a mid-IR frequency comb source. The transmitted spectra over a bandwidth of about 500 nm were recorded with an optical spectrum analyzer under various experimental conditions at different path lengths of up to ~590 m. The normalized absorption spectra were compared and fitted with simulations, yielding quantitative values of methane concentrations. A high sensitivity sensor, combining a multipass cell and wavelength modulation spectroscopy in the near infrared spectral region was designed and implemented for trace gas detection. The effective length of the multipass cell was about 290 meters. The developed spectroscopic technique demonstrates an improved sensitivity of methane in ambient air and a relatively short detection time compared to previously reported

sensors. We contributed to interstellar chemistry by determining reaction rates at a few ten kelvin temperatures employing for one reactant sympathetic cooling in an ion trap and the other reactant low temperature selection with a Stark velocity filter.

MARLAN O. SCULLY, A-1261, Texas A&M University. EXPERIMENTAL AND THEORETICAL RESEARCH INTO QUANTUM CHEMISTRY AND QUANTUM OPTICS.

This past year, we have made advances in areas including the foundations of quantum mechanics, novel applications of quantum coherence, and the development of new devices. Specifically:

- We investigated the nature of the photon – real and virtual. We found that two-photon infrared resonance can enhance coherent Raman scattering [1] which could have broad implications from coherent light generation in spectroscopic remote sensing to chemically specific imaging in microscopy. We were invited to write a feature article in Optics and Photonics News [2] where we were able to explore the less generally known role of virtual photons in phenomena ranging from the microscopic to the cosmic!

- We also demonstrated compressed sensing for single-shot compressed Raman imaging [3]. In particular, we demonstrated the identification of two similarly white substances in one image via the recovered two-dimensional array of Raman spectra making compressed hyperspectral imaging microscopy a real possibility.

- We examined the correlation versus ground state entropy for a Bose-Einstein condensate (BEC) and found that the calculation of the entropy of an ideal BEC in a three-dimensional trap reveals unusual, previously unrecognized, features of the canonical ensemble [4]. Specifically, the correlation entropy is exactly equal to the contribution from the ground state. Further investigation [5] showed for a fixed total number of particles that below the temperature of BEC, the correlation part of the entropy of an ideal Bose gas is cancelled by the ground-state contribution. Thus, allowing for use of a simplified model.

- We investigated the use of intensity correlation microscopy in combination with structured illumination to image quantum emitters that exhibit antibunching with a spatial resolution reaching far beyond the Rayleigh limit [6]. We found that for linear low-intensity excitation and linear optical detection, the resolution power was substantially enhanced.

JONATHAN T. SCZEPANSKI, A-1909, Texas A&M University. DEVELOPMENT OF CROSS-CHIRAL NUCLEIC ACID BIOSENSORS FOR DETECTION OF RNA STRUCTURES.

Significant progress has been made during the second year of this three-year award. Having successfully isolated the desired RNA-dependent aptazyme biosensor during the previous reporting period, we focused on truncating and fragmenting the aptazyme (>100 nt) in order to facilitate the eventual chemical synthesis of a bio-inert L-RNA version. Unfortunately, the aptazyme did not tolerate significant nucleotide truncations. Moreover, all attempts to fragment the aptazyme into two shorter pieces that could self-assemble into a functional RNA molecule failed. Consequently, we shifted our attention to synthesizing the full-length L-aptazyme via the "cross-chiral" ribozyme-mediated ligation of two shorter L-RNAs. This approach requires the chemical synthesis of L-RNA molecules containing a 5'-triphosphate moiety as the ligation substrate. Due to numerous technical challenges, however, chemical triphosphorylation has been limited to shorter oligonucleotides. Thus, significant effort was committed towards optimizing the chemical triphosphorylation reaction in the context of long (>50 nt) RNA molecules. To date, we have successfully achieved triphosphorylation of 50-mer oligonucleotides and are applying these methods to the construction of the desired L-RNA aptazyme biosensor. Finally, given the aforementioned difficulties associated with the synthesis of long L-RNAs, we have shifted to the use of L-DNA in our designs.

Synthesis of DNA is both less expensive and more efficient than RNA. Consequently, we anticipate that the use of L-DNA will facilitate future in vitro and intracellular studies by enabling rapid synthesis of the L-versions of our biosensors. As a proof-of-concept, we recently isolated and characterized the first L-DNA aptamer capable of binding a structured RNA (also pre-miRNA-155). In line with the goals of this Welch-funded project, we are now beginning to explore the conversion of these novel L-DNA aptamers into structure-specific RNA biosensors.

JOACHIM SEEMANN, I-1910, The University of Texas Southwestern Medical Center. BIOCHEMICAL AND STRUCTURAL ANALYSIS OF GOLGI-BASED SPINDLE ASSEMBLY ACTIVITIES.

During mitosis, importin a binds to spindle assembly factors to suppress their microtubule nucleation activity. TPX2 is an essential spindle assembly factor that is silenced by importin a. We previously discovered that microtubule polymerization activity of TPX2 is locally activated at the Golgi by GM130. GM130 sequesters importin a from TPX2, which in turn activates TPX2 to initiate local spindle microtubule formation on the Golgi to facilitate the proper partitioning of the Golgi into the daughter cells. We showed that GM130 binding to importin a depends on the mitotic phosphorylation of Ser25 in GM130. In this funding period, we found that mitotic phosphorylation of importin a is further required to enable this interaction. We first identified the mitotic phosphorylation site in importin alpha at Ser62 by quantitative mass spectrometry and showed that S62 phosphorylation is required for GM130 binding, which is an upstream requirement for local microtubule assembly on the Golgi. Functional studies then showed that S62A mutant cells became mitotically arrested and died after prolonged arrest. Consistently, microinjection of recombinant S62A importin alpha into early mitotic cells also triggered mitotic arrest.

Together our results show that phosphorylation of importin a is essential for GM130 binding to mediate proper spindle assembly and thereby for mitotic progression.

LAURA SEGATORI, C-1824, Rice University. SYNTHESIS AND CHARACTERIZATION OF BIO-INSPIRED NANOPARTICLES WITH AUTOPHAGY-MODULATING PROPERTIES.

Nanoparticles with controllable and precisely tunable aggregation properties were synthesized and their functional interaction with the autophagy-lysosome systems characterized. Carboxylated polystyrene NPs (100nm) were coated with multi-domain peptides. The sequence of multi-domain peptides was altered to assess the effect of the peptide on the nanoparticle aggregation properties. Specifically, we identified a multi-domain peptide that induces nanoparticle self-assembly in the presence of multivalent ions and a control peptide that does not result in nanoparticle self-assembly. The resulting nanoparticles were found not to self-assemble when disperse in cell culturing medium.

We evaluated a series of markers of the autophagy system in cells treated with nanoparticles coated with the multi-domain peptides and established design rules of aggregation-prone nanoparticles with autophagy-modulating properties. We established a method to render 3-D surfaces of the nanoparticle signal from confocal Z-stack files and quantify the formation and size of aggregates within the cells. This method makes it possible to correlate markers of the autophagic response to the extent of intracellular nanoparticle aggregation.

We found that the peptide-coated nanoparticles cause increase in the activity of the transcription factor EB, a master regulator of lysosomal biogenesis and autophagy, as a function of their aggregation propensity. This increase correlates with the volume of the nanoparticle aggregates upon cellular uptake. We also found that the aggregation properties of the nanoparticles affect the biogenesis of autophagosome vesicles and clearance of autophagic cargo.

These results provide insights on the design rules of nanoparticles with tunable autophagy-modulating properties and establish precise correlations between the aggregation propensity of nanoparticles and markers of the autophagy-lysosome system.

LIBO SHAN, A-1795, Texas A&M University. BIOCHEMICAL AND REGULATORY CONSTRAINTS OF IMMUNE SENSORS.

Pathogen- or microbe-associated molecular patterns (PAMPs/MAMPs) are detected as non-self by host pattern recognition receptors (PRRs) and activate pattern-triggered immunity (PTI). Collectively, PTI contributes to host defense against infections by a broad range of pathogens. PRRs are receptor-like kinases (RLKs) or receptor-like proteins (RLPs) in plants, many of which play roles in plant growth and development. We have identified ANXUR1 (ANX1), a malectin-like domain-containing receptor-like kinase, together with its homolog ANX2, as important negative regulators of immune receptor complexes, which is uncoupled from their function in plant sexual reproduction. In addition, we revealed a previously unrecognized mechanism that BR ligand-induced recruitment of E3 ligases into the BRI1 receptor complex to attenuate the signaling via ubiquitination and intracellular degradation. Furthermore, we have collaborated with the other groups and demonstrated a multi-protein receptorsome consisting of different RLKs, RLPs and receptor-like cytoplasmic kinases (RLCKs) in regulating plant immunity, and nuclear role of a RLCK in defense hormone regulation in immunity. We have contributed several comprehensive review articles and commentary articles in summarizing the remarkable progress in this field.

BRYAN F. SHAW, AA-1854, Baylor University. THE DARK SIDE OF "WILD TYPE" Cu, Zn SOD1 IN MOTOR NEURON DISEASE: METAL SNATCHER OR PRION TEMPLATE?

Major Research Highlight: This past May (2018), our Welch-acknowledged paper was featured on one of the covers of *Angewandte Chemie*! This paper was also designated by the editor as a "Very Important Paper". You can see the cover at this URL:

<https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.201803479>. This paper was the first to detect and directly measure "charge regulation" during electron transfer in proteins. In short, we measured the net electrostatic charge of a few different metalloproteins before and after the addition of a single electron. We find that some of the proteins are capable of regulating their net charge, that is, the pKa of several residues (distal to the metal center) change in response to the new electrostatic environment. This adjustment in pKa requires work and this work either contributes to the outersphere reorganization energy term (per Marcus theory) or the redox potential of the electron transfer process. Other progress: We have used fluorescence spectroscopy to determine the effect of metal free WT SOD1 on the rate of aggregation of two ALS mutant proteins, D101N and H46R SOD1, that do not fibrillize during in vitro assays. We have found that the metal free WT SOD1 protein does not necessary promote the aggregation of metal free ALS mutant SOD1, that is the presence of WT SOD1 does not uniformly affect the rate of aggregation of ALS mutant SOD1. Contrary, we have found, using mass spectrometry and capillary electrophoresis, that metal free WT SOD1 can "steal" metal ions from fully metallated ALS mutant SOD1. This is one mechanism by which the WT SOD1 protein can increase the aggregation propensity of mutant SOD1.

JASON B. SHEAR, F-1331, The University of Texas at Austin. DEVELOPMENT OF MICRO-3D-PRINTED OPTICAL FIBER PROBES FOR REMOTE CHARACTERIZATION OF COMPLEX BIO-ENVIRONMENTS.

We developed capabilities for trapping bacteria within micro-3D (μ 3D) printed protein-based structures on depolyable (105- μ m core) optical fibers. Pathogenic *P. aeruginosa* cells were suspended in fabrication reagent containing porcine gelatin and bovine serum albumin (BSA), which were promoted to undergo intermolecular crosslinking via multiphoton excitation of the photosensitizer, Rose Bengal (RB; 7 mM) using focused femtosecond laser light in a plane-by-plane digital masking procedure. Gelatin, BSA, and RB concentrations were optimized for microstructure physical integrity and adhesion to fiber tips without toxicity. The optical fiber, secured within a chuck, was mounted to a three-axis micropositioner on the stage of an inverted microscope. Fabrication was performed by focusing femtosecond laser light to the downward-facing fiber tip submersed in fabrication reagent, positioned to a plane appropriate for fabrication. After reagent gelation, it was possible to enclose stationary cells using μ 3D printing. Using this approach, we were able to trap, and subsequently incubate cells with normal division rates in both small (1.5 pL) and larger (~19 pL) cylinders. These results validate that bacterial microclusters of defined size, shape, and composition can be localized on a fiber tip under micropositioner control, while maintaining chemically interactivity with their surroundings.

Further, we have begun construction of a laser-based detection system for use with the optical fiber for fluorescence analysis of μ 3D printed cellular response, which we anticipate implementing in the coming months. Finally, μ 3D printing and bacterial analysis capabilities enabled by this project have resulted in a published report on effects of inter-cluster distances on bacterial behavioral (in PNAS), a submitted report (accepted in 6/2018) on effects of differing antibiotic treatments on viability (to Analyst), and a manuscript nearing submission on nitric oxide detection (to JACS).

MATTHEW SHELDON, A-1886, Texas A&M University. HOT CARRIER UP-CONVERSION LUMINESCENCE IN NANOCRYSTAL HETEROSTRUCTURES.

A major breakthrough in the past year has been the discovery and quantitative analysis of single photon up-conversion luminescence using hybrid cesium-based inorganic CsPbX (X = I, Br,Cl) perovskite NCs with or without Au deposition, after developing the expertise to control the metal deposition last year.

This is an especially intriguing material system due to the tunability of band-edge emission across the entire visible spectrum using straight-forward compositional modification during synthesis, as well as unusually high quantum yield at unity within our instrumental error, as prepared. Remarkably, single photon up conversion, also called anti-stokes photoluminescence, occurs with quantum yield over 70% in our studies (Chem. Comm. 2018). This means these nanoparticles may also be a champion materials system for optical cooling, as the up-converted photon is produced by scavenging heat via phonon scattering. Ongoing studies are determining the limits of the optical cooling power, as well as more detailed insight into the electron-phonon coupling that makes the up-conversion possible. Further, initial experiments suggest that the plasmonic enhancement of the anti-stokes scattering (similar mechanically to SERS phenomena) may further improve the efficiency of optical cooling.

In parallel, our computational analysis of the optical behavior of the plasmonic Au regions in close contact with semiconductors has enabled us to provide comprehensive optical analysis of a variety of metal- semiconductor systems via collaboration, as well as publish a new manuscript outlining opportunities for all-metal optical power conversion based on tunneling of hot carriers in plasmonic nanostructures (ACS Photonics, 2018). We show that optical power conversion efficiencies can rival or out-perform photovoltaic-based approaches when photothermalization also provides a thermal gradient across the metal interface. We are currently measuring electrical devices guided by this analysis.

A. DEAN SHERRY, AT-0584, The University of Texas at Dallas. SHIFT REAGENTS FOR MRI DETECTION OF SPECIFIC METABOLITES.

The binding of biologically important molecules to paramagnetic lanthanide DO3A-type complexes offers new avenues for molecular imaging of such species. Lactate, for example, is overproduced in most cancers yet methods to quantify lactate production *in vivo* are lacking, especially methods that can distinguish intracellular lactate from extracellular lactate. We have shown that the paramagnetic shift reagent, EuDO3A, forms a bidentate complex with lactate even in the presence of variety of competing biological anions. When weakly bound to EuDO3A, lactate was easily detected via CEST-MRI by selective activation of the highly shifted, exchanging lactate –OH proton. Preliminary MRI studies of mice bearing a tumor xenograft show that EuDO3A can be safely injected into animals and that lactate can be imaged in the extracellular space of tumors before the agent is cleared via renal filtration. Introduction of chiral centers on the pendant arms of DO3A resulted in several new chiral SRs such as Eu or YbDO3A- tris(alanine) and Eu or YbDO3A-tris(aspartate). These new chiral shift reagents easily discriminate D- and L-lactate by CEST-MRI. This is an important finding because it has been reported that some cancer cell lines generate both D-lactate using a mitochondrial form of LDH and L-lactate using the more common cytosolic form of LDH. Given that little is known about the biological reasons for D-lactate production by mitochondrial LDH in some cancer cells, these new chiral shift reagents combined with CEST-MRI offers the possibility of imaging production of both D- and L-lactate in tumors *in vivo*.

XIAOBING SHI, G-1719, The University of Texas M.D. Anderson Cancer Center. STRUCTURE AND FUNCTIONS OF A NOVEL HISTONE ACETYLATION READER.

We have previously reported the YEATS domain as a novel histone acetylation reader (Cell 2014). Recently, we found that the YEATS domain of ENL protein recognizes acetylation on histone H3K27 and H3K9. which is required for disease maintenance in acute myeloid leukaemia (AML) (Nature, 2017). However, the functional importance of other YEATS domain-containing proteins in human cancer remains largely unknown. We found that the YEATS2 gene is highly amplified in human non-small cell lung cancer (NSCLC) and is required for cancer cell growth and survival. YEATS2 binds to acetylated histone H3, with strong preference to H3K27. Depletion of YEATS2 or disruption of the interaction between its YEATS domain and acetylated histones reduces the ATAC complex-dependent promoter H3K9ac levels and deactivates the expression of essential genes that are important for cancer cell growth and survival. Taken together, our study identifies YEATS2 as a histone H3K27ac reader that regulates a transcriptional program essential for NSCLC tumorigenesis. This work has recently been published on Nature Communications, 2017. In a similar study, we found that another YEATS domain protein, GAS41, binds to histone H3 acetylated on H3K27 and H3K14. Depletion of GAS41 or disruption of the interaction between its YEATS domain and acetylated histones impairs the association of histone variant H2A.Z with chromatin, and consequently, suppresses cancer cell growth and survival both *in vitro* and *in vivo*. Overall, our study identifies GAS41 as a histone acetylation reader that promotes histone H2A.Z deposition in NSCLC. This work has recently been published in Genes & Development, 2018.

CHIH-KANG SHIH, F-1672, The University of Texas at Austin. TAILORING ELECTRONIC AND EXCITONIC STRUCTURES OF 2D MATERIALS.

- Development of a universal approach to grow atomically smooth epitaxial Ag films with precise thickness control from a few monolayers to optically thick regime, overcoming the limitations of existing methods. We will submit the paper for publications shortly.
- We have investigated the strain distributions and their influence on electronic structures of WSe₂-MoS₂ laterally strained heterojunctions. We determined, for the first time a 2D strain tensor at a nanometer resolution and achieved direct electronic structure mapping and determine quantitatively how strain impacts the electronic structures of a lateral heterojunction.
- We have developed a double-coil apparatus designed to operate in ultra-high vacuum to measure the complex conductivity (including real part and imaginary part) of metallic thin films.
- We have successfully tailored a lateral multi-heterojunction of atomically thin semiconductors (more specifically monolayer WS₂/WS₂(1-x)Se_{2x}/WS₂ multijunction) via direct growth by chemical vapor deposition. By using this structure, we have demonstrated an enhancement of local photoconductivity by two orders of magnitude over pure WS₂.

QIMIAO SI, C-1411, Rice University. THEORETICAL STUDIES OF ELECTRONIC DYNAMICS AND CORRELATIONS IN CARBON-BASED AND RELATED LOW DIMENSIONAL STRUCTURES.

This year's progresses are as follows, resulting in 14 papers published or accepted and 2 submitted:

- Electronic dynamics and magnetic defects in beyond-graphene low-dimensional structures. Such systems host novel electronic states. We advanced on the phase diagrams of theoretical models defined on the graphene-type honeycomb and related lattices, with spin-orbit coupling included. In particular, linearly dispersing Dirac (and Weyl) nodes robustly arise in the electronic excitation spectrum, and are shown to strongly affect the electrons' dynamics and their coupling to magnetic defects. Our studies also led to several collaborations with experimental groups. Especially, in collaboration with Prof. Kono's group at Rice and a collaborator from Vienna, we acquired preliminary results on dynamical omega over T scaling in the optical conductivity of newly made heavy fermion MBE films, thereby opening up an entirely new frontier. Five papers were published or accepted (including one each in PNAS and Nature Commun.) and one more was submitted to PNAS.
- Many-body effect of quantum criticality. This is a prototype many-body feature of low-dimensional nanostructures, where quantum fluctuations are particularly pronounced. We demonstrated unusual dynamical and transport properties in three classes of – respectively magnetic, correlation-driven insulating, and metallic -- model systems of high relevance to experiments. Five papers were published, including one in (the recently launched Nature-partner journal) npj Quantum Materials.
- Superconductivity driven by electron correlations. This is an integral part of work on many-body effects, key to the electronic properties of low-dimensional structures. We made large efforts to elucidate the interplay between superconductivity and other types of electronic orders. Four papers were published (including one each in PNAS and Physical Review Letters) and one more was submitted to Physical Review Letters.

DANIEL J. SIEGWART, I-1855, The University of Texas Southwestern Medical Center. DESIGN AND SYNTHESIS OF ACTIVATABLE pH-RESPONSIVE WATER SOLUBLE DYES FOR BIOMEDICAL IMAGING.

We have worked on chemical elucidation of design rules and structure-activity relationships (SAR) for the proposed BODIPY-based imaging probes. We anticipate that this will provide control over micrometastasis tracking with high tumor-to-background contrast. Thus far, the proposed chemical routes have been successful. We have synthesized a series of modular water-soluble probes with different PEG molecular weights. These probes have been purified and characterized by various physical characterization methods including nuclear magnetic resonance (NMR) spectroscopy, mass spectroscopy, and fluorescence measurements. The quantum yields have also been calculated. Early efforts have already allowed imaging of subcutaneously implanted human xenograft tumors in mice. The uptake of the initial set of probes into tumors strongly correlates with PEG length. This is an encouraging finding that suggests potential validation of our hypotheses and experimental approach. Going forward, we will continue syntheses and physical chemistry measurements. In the next 1-2 years, we will also develop metastases models of cancer and proceed with in vivo tumor imaging evaluation. We have published a series of manuscripts thanks to funding of this grant.

ALEXEI V. SOKOLOV, A-1547, Texas A&M University. ULTRAFast COHERENT MOLECULAR SPECTROSCOPY WITH SPATIALLY AND TEMPORALLY SHAPED ELECTROMAGNETIC FIELDS.

We explore possibilities for controlled/tailored broadband coherent Raman generation. We cross two femtosecond laser pulses (pump and Stokes) in a Raman-active crystal and study the effects of input pulse shapes, as well as transverse-spatial beam shapes, on the generation process. We recombine the generated sidebands, with controllable phases, in order to synthesize precisely tailored waveforms for ultrafast spectroscopic studies of molecules. We determine the degree to which the output spectrum can be controlled by the input beam shape, by using a liquid-crystal light modulator to produce arbitrary pump beam structures. We perform programmable phase-only spatial optimization in order to influence the supercontinuum generation process, and show that controlled spectral broadening is possible without loss of input energy. In a separate set of experiments, we study applications of coherent Raman anti-Stokes scattering (CARS) to micro-spectroscopy and chemical mapping, and demonstrate video-rate imaging by femtosecond adaptive spectroscopic technique (FAST) CARS aided by optimized picosecond supercontinuum generated in a photonic-crystal fiber. We discuss the possibility to combine coherence and plasmonic nano-structure enhancements in surface-enhanced and tip-enhanced FAST CARS techniques, where laser pulse shaping of near-field excitations

plays an important role. This work will lead to the development of nano-spectroscopic tools for studies of molecular structure and dynamics, as well as surface chemistry.

DONG HEE SON, A-1639, Texas A&M University. HOT ELECTRONS GENERATED FROM UPCONVERSION IN DOPED QUANTUM DOTS.

In this project year, our research focused on the following. (1) Expanding the range of host perovskite materials and imposing quantum confinement for more efficient hot electron generation (2) Developing the method to co-dope Cu ions in addition to the Mn to enhance the efficiency of hot electron generation. Although doping Mn in CsPbCl₃, achieved in the previous year, is much easier than in CsPbBr₃ or CsPbI₃, its high bandgap and relatively high defect density made it less ideal as the host of Mn-doped nanocrystals generating hot electrons. However, doping in CsPbBr₃ or CsPbI₃ is much more challenging since doping Mn in these hosts is thermodynamically much more unfavorable than doping in CsPbCl₃. Here, we achieved the synthesis of Mn-doped CsPbBr₃ nanocrystals via the formation of an intermediate monolayer structure before the hot-injection of the Cs precursor, which contains the same Mn-Br coordination present in Mn-doped CsPbBr₃ nanocrystals. The successful Mn doping in CsPbBr₃ nanocrystal host expanded the range of solar spectrum that can be harvested for hot electron generation. We also succeeded in producing perovskite host with strong and controlled quantum confinement. The lack of a robust method for producing quantum dots with controlled size and high ensemble uniformity has been one of the major obstacles in exploring the useful properties of excitons in CsPbX₃ quantum dots. Here, we developed a new synthesis approach that enables the precise control of the size based on the equilibrium rather than kinetics, producing CsPbX₃ quantum dots nearly free of heterogeneous broadening in their exciton luminescence. Finally, we successfully co-doped both Mn and Cu in the CdS/ZnS quantum dots, where the presence of Cu can prolong the lifetime of electron and increase hot electron generation efficiency. The co-doped quantum dots exhibited nearly an order of magnitude increase in hot electron photoemission current compared to singly doped quantum dots with Mn.

ZHOU SONGYANG, Q-1673, Baylor College of Medicine. BIOCHEMICAL STUDIES OF PATHWAYS AND COMPOUNDS THAT MODULATE TELOMERE LENGTH.

While studying TPP1-mediated telomerase recruitment, we identified the Shwachman-Bodian-Diamond syndrome (SBDS) gene product as a novel protein that interacts with TPP1. We found that SBDS deficiency led to disrupted telomerase recruitment and telomere shortening. We further showed that SBDS functioned via its interaction with TPP1 by a cell cycle-dependent mechanism. In particular, two SBDS point mutations found in patients resulted in specific decreases in telomerase activities recruited by TPP1. Collectively, these results indicate that telomere loss in SDS patients is caused by diminished TPP1-mediated recruitment of telomerase and suggest possible new therapeutics that may help combat SDS.

Telomere ends adopt higher-order structures that must be resolved for successful replication. BUB3 and BUB1 are core components of the key mitotic surveillance mechanism spindle assembly checkpoint (SAC), which prevents anaphase onset until successful and proper attachment of all chromosomes to microtubules. We showed for the first time that both BUB3 and BUB1 could localize to telomeres. Loss of BUB3 or BUB1 led to multiple telomere abnormalities including stalled telomere replication forks and reduced telomere DNA replication, as well as telomere fragility, loss, and shortening. We found that BUB3, and in turn BUB1, was recruited to telomeres during S phase through direct interactions with TRF2. And BUB1 phosphorylates TRF1 at S296 and facilitates its recruitment of BLM. When we added 2OH-BNPP1, a BUB1-specific small-molecule inhibitor to synchronized HeLa cells, increased telomere defects such as MTS and telomere loss were observed, indicating that inhibition of BUB1 kinase activity during S phase clearly led to disrupted telomere replication. Our findings support an essential role for the BUB3-BUB1 complex in resolving telomere replication problems during S phase, and highlight the link between telomerase/telomeres with mitotic surveillance pathways.

MIHAELA C. STEFAN, AT-1740, The University of Texas at Dallas. SEMICONDUCTING BLOCK COPOLYMERS CAPABLE OF ACTUATED CHANGES OF OPTO-ELECTRONIC PROPERTIES.

A new pyrrole building block was synthesized in our group, and it will be used to generate liquid crystalline semiconducting polymers. The pyrrole building block is challenging to synthesize but the expected optical and electronic properties are excellent. The smallest S, N-heteroacene and O, N-heteroacene; thieno[3,2-b]pyrrole and furo[3,2-b]pyrrole were used to generate donor-acceptor-donor type organic semiconducting small molecules. Since both building blocks are highly electron-rich, thiophene flanked 5,6-difluorobenzo[c][1,2,5]thiadiazole was employed as the central electron-withdrawing unit. The small molecule containing thieno[3,2-b]pyrrole (TP-FBT2T-TP) exhibited moderate hole mobilities (10⁻³ cm² /V s) irrespective of the annealing temperature. In contrast, the small molecule bearing furo[3,2-b]pyrrole was completely inactive in field-effect transistors. Devices based on small molecules with thieno[3,2-b]pyrrole exhibit near-ideal transistor characteristics. All the devices fabricated from TP-FBT2T-TP showed near-ideal transistor curves with low leakage currents and clear saturation regimes. Subthreshold swings up to 0.7 V/dec were obtained for these devices. Most of all, the ID1/2 vs VD curves did not display non-linearity that generally introduce errors when extracting mobilities from transfer curves. We are now introducing the thieno[3,2-b]pyrrole (TP-FBT2T-TP) building block in liquid crystalline semiconducting polymers with pyrene mesogens.

WU-PEI SU, E-1070, University of Houston. DIRECT PHASING IN MACROMOLECULAR CRYSTALLOGRAPHY.

We have developed a theoretical scheme (the so-called HIO (hybrid-input-output) method) for phasing a protein crystal. It is based on the fact that the electron density in the solvent region is a constant. It turns out that for high-solvent content crystals this constraint is strong enough to allow the phases of the reflections to be solved. Empirically we find that for solvent fractions higher than 70% there is a good chance that the crystal can be phased, therefore in

that case a protein structure can be solved without preparing a derivative crystal. As a recent trial calculation, we have solved the structure of a membrane protein, which typically has a high solvent content and the crystal usually does not diffract well. Although an atomic model of the structure can be obtained only for data with a resolution higher than 3.5 Angstroms, we found that for data truncated between 4-7 Angstroms, useful information such as secondary structures can still be extracted.

The requirement of high-solvent content severely limits the usefulness of our algorithm, as the solvent content of most crystals lies between 40 and 60%. Fortunately another feature of a protein crystal comes to the rescue. A significant fraction of protein crystals exhibit non-crystallographic symmetry (NCS), which effectively reduces the degrees of freedom of protein with respect to the solvent, rendering the phase problems solvable again. We have demonstrated this by carrying out trial calculations of structures with three fold and two fold symmetry axes and also a structure with translational NCS. This is a very important progress, as at least one third of all protein crystals possess NCS. Thus our algorithm will become a practical tool for crystallographer when it is properly developed. Right now we need to assume an accurate knowledge of the NCS, such as the location of the symmetry axis. It might be possible to determine the NCS parameters iteratively from unknown or approximately values.

JEFFREY J. TABOR, C-1856, Rice University. NEXT-GENERATION ANTIBIOTICS: HIGH THROUGHPUT DISCOVERY OF INHIBITORS OF PATHOGENIC BACTERIAL TWO-COMPONENT SYSTEMS.

We have discovered two highly promising lead compounds that inhibit SaeRS, the major virulence pathway in methicillin-resistant *Staphylococcus aureus* (MRSA), a major problematic pathogen. In particular, we used our DNA binding domain swapping method to functionally express SaeRS in the common laboratory bacterium *Bacillus subtilis*. Using this more convenient host, we screened the pathway against ~1,500 compounds from the NIH chemical diversity library. We discovered approximately 10 hits and validated each with a series of control experiments. We then collaborated with Eric Skaar's group at Vanderbilt university to validate the ability of these hits to inhibit SaeRS function in MRSA. The Skaar group showed that two of the ten, NSC97920 and NSC33005, strongly and reproducibly inhibit SaeRS in MRSA. We are now making plans to evaluate their effectiveness in combating MRSA infection in animal studies.

The power of our technology is that it can be applied to dozens of two-component systems and numerous pathogens. Thus, we are replicating our approach for other systems from *Salmonella* and other major pathogens.

VINCENT S. TAGLIABRACCI, I-1911, The University of Texas Southwestern Medical Center. NOVEL BACTERIAL SPORE COAT PROTEIN KINASES.

Although we continue to study the CotH family of kinases, our research has shifted gears this past reporting period. We have discovered that the uncharacterized pseudokinase selenoprotein O (SeIO), is in fact an active enzyme, but transfers AMP to proteins rather than phosphate like other protein kinases. This work has received positive reviews at Cell and we have addressed the minor concerns and resubmitted the manuscript, which we anticipate will be accepted for publication. SeIO contains the 21st genetically encoded amino acid selenocysteine and regulates the activity of redox active proteins. Importantly, SeIO appears to protect cells from oxidative stress. This work has far reaching implications, not only in cell signaling, but also in the regulation of redox biology, which plays an important role in numerous human diseases.

During this reporting period, we have also discovered a kinase family distantly related to the CotH kinases. This family, named HopBF1, is found in several animal and plant pathogens and is a Type 3 secretion system effector protein. We have identified host cell HSP90 as the HopBF1 target substrate and discovered a novel "betrayal" mechanism by which bacterial effectors modulate host immunity. HSP90 is a molecular chaperone that facilitates the folding of innate immune receptors and ~60% of the human kinome. We have discovered that HopBF1 adopts a minimal protein kinase-like fold that is recognized as a host cell HSP90 client. As a result, HopBF1 phosphorylates and inactivates HSP90 to compromise folding of proteins, including innate immune receptors. Importantly, we show that HopBF1-dependent phosphorylation of HSP90 is sufficient to induce tissue collapse and necrosis in plants infected with the bacterial pathogen *Pseudomonas syringae*. This paper has recently been submitted to Science.

UTTAM K. TAMBAR, I-1748, The University of Texas Southwestern Medical Center. STEREOSELECTIVE TRANSFORMATIONS OF DIENES.

Recently, we published the regioselective and diastereoselective aminoarylation and aminothiolation of 1,3-dienes. We utilized *N,N'*-Bis(benzenesulfonyl)sulfur diimide to selectively functionalize 1,3-dienes via a [4+2] cycloaddition to generate a cyclic sulfinamide. This intermediate was then treated with a copper catalyst and aryl Grignard reagents to generate aminoarylation products with three new functional groups (an aryl ring, a sulfonamide, and a Z-olefin). With unsymmetrical 1,3-dienes as substrates, the products were generated in high regioselectivity and diastereoselectivity. Alternatively, the [4+2] cycloadduct was treated with a copper catalyst and aliphatic Grignard reagents to generate aminothiolation products with three new functional groups (a thioether, a sulfonamide, and a Z-olefin). In addition to providing access to synthetically challenging polyfunctional compounds, our selective reactions with 1,3-dienes represent important discoveries in the fundamental reactivity of unsaturated hydrocarbons.

During this grant year, we made progress on Aim 1 of the Grant by generally studying enantioselective reactions with unsaturated compounds. For examples, we obtained promising preliminary data for the catalytic enantioselective propargyl amination of terminal alkynes, based on the unique reactivity of *N,N'*-Bis(benzenesulfonyl)sulfur diimide.

During this grant year, we made progress on Aim 2 of the Grant by developing other classes of reactions with unsaturated starting materials. We discovered a catalytic reaction for the selective and sequential replacement of three C-H bonds at the allylic position of propylene with different carbon groups

derived from Grignard reagents. N,N'-Bis(benzenesulfonyl)sulfur diimide is utilized as the terminal oxidant. This method provides a new approach to diverse and complex products with quaternary carbon centers that can be generated from simple and abundant feedstock chemicals.

YIZHI JANE TAO, C-1565, Rice University. STRUCTURAL AND FUNCTIONAL STUDIES OF VIRAL POLYMERASES.

Hepatitis B virus (HBV) causes human liver infection that may lead to serious health issues such as cirrhosis and liver cancer. The replication process of HBV is unique as it relies on reverse transcription to produce a double-stranded DNA genome. To gain a better understanding of the HBV replication mechanisms, our laboratory has made extensive efforts to express, purify and crystallize the multifunctional polymerase proteins from human HBV, homologous HBVs isolated from monkey, bat, duck, fish and frog, together with two non-enveloped fish viruses recently discovered (i.e. Rockfish Nakednavirus and Sockeye Salmon Nakednavirus). Several single-domain and multi-domain constructs have been identified to produce milligram-levels of soluble proteins. X-ray crystallography and cryo-electron microscopy are currently being pursued for structural analysis.

Meanwhile, we have made several major advances in our molecular characterization of the delta protein from the nematode-infecting Orsay virus. We have found that: (1) authentic Orsay virion contains capsid fibers, suggesting that the CP-delta protein is incorporated into infectious particles; (2) the other two nematode viruses, Le Blanc and Santeuil, also encode a homologous delta protein of a filamentous shape; (3) free delta protein of Orsay interacts with the intestinal terminal web to facilitate non-lytic viral exit at the apical side of the worm intestine during infection; (4) several worm host proteins have been identified by both pull-down and yeast two-hybrid experiments to interact with the Orsay delta protein.

We have also shown that mammalian TRIM25 directly binds to the influenza A virus ribonucleoprotein complex to specifically blocks influenza A virus replication in a manner that is independent of the RIG-I mediated interferon induction pathway. The restriction factor activity of TRIM25 likely plays a role in regulating cross-species transmission of influenza viruses.

DAVID TAYLOR, F-1938, The University of Texas at Austin. CHEMICAL INSIGHTS INTO SUBSTRATE CLEAVAGE BY CRISPR-CASCADE.

Bacterial adaptive immunity utilizes RNA-guided surveillance complexes composed of CRISPR (clustered regularly interspaced short palindromic repeats)-associated (Cas) proteins together with CRISPR RNAs (crRNAs) to target foreign nucleic acids for destruction. Cas9, a type II CRISPR-Cas effector complex, can be programmed with a single guide RNA that base-pairs with the target strand of dsDNA, displacing the non-target strand to create an R-loop, where the HNH and RuvC nuclease domains can cleave opposing strands. Cas9 has been repurposed for a variety of important genome engineering applications. While many structural and biochemical studies have shed light on the mechanism of Cas9 cleavage, a clear unifying model has yet to emerge. Our detailed kinetic characterization of the enzyme reveals that DNA binding is reversible, R-loop formation is rate-limiting, occurring in two steps, one for each of the nuclease domains. Although the HNH nuclease activity is stimulated by Mg²⁺ with a single measurable K_d, the RuvC activity requires two distinct Mg²⁺ binding events. The specificity constant for cleavage is determined through an induced-fit mechanism as the product of the equilibrium binding affinity for DNA and the rate of R-loop formation.

THOMAS S. TEETS, E-1887, University of Houston. FINE TUNING OF MOLECULAR CATALYSTS AND PHOTSENSITIZERS VIA SYNTHETIC ALLOSTERY.

The PI's major efforts during the past year involved developing new synthetic strategies for cyclometalated iridium complexes with desirable properties, overcoming the synthetic challenges that primarily arise from the substitutional inertness of iridium(III). The PI's group has discovered two new classes of cyclometalated iridium complexes with acyclic diaminocarbene (ADC) ancillary ligands, using nucleophilic addition to coordinated isocyanides as an unconventional strategy to access these compounds. Many of these exhibit brilliant blue luminescence with exceptional quantum yields when immobilized in polymer films, and efforts are underway to optimize these complexes even further to generate high-purity, deep-blue emission.

Other efforts in the group focused on red-emitting bis-cyclometalated iridium complexes with electron-rich, nitrogen-containing nitrogen ancillary ligands. This effort has resulted in two complementary designs for champion red-emitting compounds, in addition to increased fundamental insights into structure-proper relationships in these compounds. Using related design elements, the PI's group has discovered a new class of potent cyclometalated iridium photoreductants, made additional synthetic modifications to these compounds to further optimize their excited-state reactivity, and begun applying them in photoredox transformations of difficult substrates.

A third thrust in the PI's research group has been the coordination chemistry of electron-deficient β -diketiminates and formazanate ligands with third-row transition metals. Highlights of the fluorinated β -diketiminates include ligand-based redox activity and red to near-infrared luminescence in platinum complexes. With formazanates, electronic structures of heteroleptic platinum formazanates have been elucidated, structurally dynamic iridium formazanates are currently being pursued, and the proton-coupled reduction of formazanates to azo-iminates has also been discovered.

JONATHAN R. TERMAN, I-1749, The University of Texas Southwestern Medical Center. CHEMISTRY AND ENZYMOLOGY OF MICAL FAMILY OXIDOREDUCTASES.

The chemical modification of specific amino acid residues is a critical means to alter the biological activity of proteins. Post-translational modifications such as the kinase-mediated phosphorylation of amino acids alters the activity of specific proteins in a reversible manner. Recently, the oxidation of specific amino acids has also become appreciated as another key mechanism in which to modify protein function – but the enzymes that mediate these oxidation-reduction (Redox) reactions are poorly defined. Interestingly, we have identified a novel family of proteins, the MICALs, who are similar to Redox

enzymes. Our investigations of these proteins over the past few years with the support of the Welch Foundation has revealed that Mical stereo-specifically oxidizes a polymerized form of the cellular protein actin to generate actin Met-44-R-sulfoxide – revealing that the conversion of specific Met/Met(R)O residues is a precise means to control protein function. Our work supported by the Welch Foundation has also revealed that this new mechanism is reversible – and that this is accomplished by an enzyme family called MsrBs/SeLRs. Thus, we have identified a new reversible post-translational modification and Redox regulatory system – and over the past year we have been investigating how this new Redox biochemical system 1) fits in with classically studied cell-cell signal transduction pathways and post-translational modifications, 2) is conserved across species, and 3) is involved in diseases. Our published work in the past year reveals that this reversible Redox regulatory system interacts with multiple well-known growth factor signal transduction pathways and that this biochemical system and mechanism is conserved from invertebrates to humans. Our results also reveal that this Mical Redox system directly associates with tyrosine kinase-mediated phosphorylation, and altering this Redox system diminishes tumor growth and progression triggered by Abelson (Abl) kinases.

RANDOLPH P. THUMMEL, E-0621, University of Houston. CYCLOTETRAPYRIDINES AND RELATED 6-5 CHELATORS.

A structure activity relationship (SAR) study was performed on a series of Ru(II) complexes containing isomeric tetramethyl-substituted bipyridyl-type ligands. Three of the ligand systems studied contained strain-inducing methyl groups and created photolabile metal complexes, which can form covalent bonds to biomolecules upon light activation, while the fourth was unstrained and resulted in photostable complexes, which can generate $^{1}O_2$. The compounds studied included both bis-heteroleptic complexes containing two bipyridine ligands and a third, substituted ligand, and tris-homoleptic complexes containing only the substituted ligand. The photophysics, electrochemistry, photochemistry, and photobiology were assessed. Strained heteroleptic complexes were found to be more photo-active and cytotoxic than tris-homoleptic complexes, and bipyridine ligands were superior to bipyrimidine. However, the homoleptic complexes exhibited a superior ability to inhibit protein production in live cells. Specific methylation patterns were associated with improved activation with red light, and photolabile complexes were generally more potent cytotoxic agents than the photostable $^{1}O_2$ generating compounds.

A mononuclear ruthenium complex $[Ru(tpy)(bpg)H_2O]^{2+}$ bearing a bipyridine glycoluril ligand where $bpg = 4b,5,7,7a$ -tetrahydro-4b,7a-nepiminomethan-oimino-6H-imidazo[4,5-f][1,10] phenanthroline- 6,13-dione acts as a robust water oxidation catalyst (WOC) at pH = 1 using Ce(IV) as a sacrificial oxidant. The turn over number (TON) for water oxidation is found to be ~ 5 times higher than the parent complex $[Ru(tpy)(bpy)H_2O]^{2+}$ where $tpy = 2,2':6',2''$ -terpyridine; $bpy = 2,2'$ -bipyridine. The presence of intermolecular H-bonding groups and the electronic effect of the functionalized bipyridine ligand may play a significant role in water oxidation.

CHIN-SEN TING, E-1146, University of Houston. SUPERCONDUCTIVITY IN Fe-PNICTIDES AND OTHER ELECTRON-CORRELATED MATERIALS.

Motivated by recent nuclear magnetic resonance experiments (K. Matano et al., Nat. Phys. 12, 852 (2016)) which suggested the superconductivity (SC) pairing symmetry in $Cu_xBi_{1-x}Se_3$, a topological insulator at $x=0$, should be rotation-symmetry breaking and similar to that of the A-phase in liquid 3He , we explored whether the corrugated cylindrical Fermi surface of $Cu_xBi_{1-x}Se_3$ would or would not support the surface Andreev bound states (SABSs) inside the bulk SC gap of this compound. Using the band parameters which fit qualitatively the experimental Fermi surfaces, the SABSs are numerically shown to be stable and exist in the clean system for both spheroidal and corrugated cylindrical Fermi surfaces, and the zero-energy Majorana bound state is a characteristic of the SABSs. However, this result is still needed to be confirmed by future experiments. We also calculated the local density of states (LDOS) around a single Te or Se vacancy in a $Fe(Te,Se)$ or an As vacancy in $Ba(Fe_{1-x}Co_xAs)_2$ compound, and predicted the quasiparticle interference patterns in order to understand the role of Te, Se and As atoms played in these Fe based superconductors. In addition, the Larkin-Ovchinnikov (LO) state of SC Weyl metals is investigated. We found the LO states when the SC pairings are assumed to be restricted and extended respectively in the k-space are to be qualitatively different, the consequence is carefully analyzed. Furthermore, we also demonstrate theoretically how a Weyl semimetal can be obtained by irradiating a Luttinger semimetal with elliptically polarized light.

FRANK K. TITTEL, C-0586, Rice University. APPLICATION OF MID-INFRARED QUANTUM AND INTERBAND CASCADE LASER TO HIGH PRECISION TRACE GAS MONITORING.

During this grant year our research efforts were focused on improving the performance of mid-infrared trace gas sensor platforms based on two gas sensing technologies, QEPAS and LAS. We investigated different types of gas sensors for a wide range of real-world applications such as environmental and pollution monitoring as well as atmospheric chemistry [CO, CO₂, NO, CH₄, H₂CO, C₂H₅F, N₂O, NO₂, industrial applications [HCl, CH₄, C₂H₆, H₂S, SF₆, C₂H₂, agricultural applications and food industries [C₂H₄, CH₄, N₂O] and breath analysis (NO, CO, NH₃, C₂H₆, H₂S, HCN). Furthermore due to the compactness and robustness of QEPAS based sensors modules other interesting real world chemical sensing applications such as sensors deployed on drones can be envisioned. Furthermore, the QTF and micro-resonator dimensions as well as the QTF geometry influence the Q-factors and the resonance frequencies of the QEPAS spectrophone. Custom QTFs also allowed the extension of the QEPAS technique into the THz range, where, due to the fast rotational-vibrational relaxation rates, the QEPAS technique is more efficient, as demonstrated by the record NNEA factor achieved so far [$3.75 \times 10^{-11} \text{ cm}^{-1} \text{ W-Hz}^{-1/2}$]. The first demonstration of intra-cavity quartz-enhanced photoacoustic spectroscopy applied to mid-infrared NO detection using a compact bow-tie cavity design geometry resulted in a minimum detection limit of ~4.8 ppbv for NO. Exploiting novel micro-resonator configurations, capable of increasing the QEPAS signal-to-noise ratio by two orders of magnitude was achieved by the utilization of QTF overtone flexural modes. A dual-gas QEPAS sensor system by means of frequency division multiplexing techniques was developed. Two beams from two independently modulated lasers are focused at two different positions between the QTF prongs to excite both the QTF fundamental and 1st overtone flexural modes simultaneously.

ZACHARY J. TONZETICH, AX-1772, The University of Texas at San Antonio. EARTH-ABUNDANT TRANSITION METAL CATALYSTS SUPPORTED BY PINCER LIGANDS.

The previous grant cycle was our most productive to date in the area of pincer chemistry resulting in three publications, one of which was featured on the inside cover of Dalton Transactions. We have now established the basic coordination chemistry of the pyrrole-based pincer ligand, RPNP (PNP = anion of 2,6-bis(dialkylphosphinomethyl)pyrrole); R = tBu, Cy, or Ph) with both Fe and Co. In the course of our studies, we revealed that the ligand is capable of supporting complexes in a variety of oxidation states, spin states, and coordination numbers. Most recently, we demonstrated the first ligand-based redox chemistry of the RPNP ligand. In a just-published manuscript, we show how treatment of both Co and Ni complexes of the tert-butyl-substituted variant of the RPNP ligand with benzoquinone results in net dehydrogenation of the pincer backbone resulting in a new, fully p-conjugated ligand we refer to as dehydro-PNP (dPNP). Cobalt complexes of dPNP show marked differences in their redox potentials and reactivity compared with the parent system. Most surprisingly, these differences come about from enhanced basicity at the nitrogen donor atom. This counter-intuitive result whereby the formally oxidized dPNP ligand becomes a more electron-rich donor is rationalized by recognizing that dearomatization of the pyrrole ligand liberates the nitrogen lone pairs rendering the atom more basic. We leverage the new properties of the dPNP to prepare hitherto unobtainable complexes of cobalt(II) including an ethyl complex. We also demonstrate the conjugated nature of the dPNP ligand by generating the reduced p- radical anion. Looking ahead, we are near completion on two manuscripts detailing the mechanisms of aldehyde decarbonylation by Co(I) and catalytic hydrosilylation by Fe(II). Both of these studies validate our strategy of employing kinetically stabilizing ligands to gain unprecedented insight into the mechanisms of organic transformations mediated by earth-abundant metals.

THOMAS M. TRUSKETT, F-1696, The University of Texas at Austin. LIQUIDS NEAR INTERFACES: SINGLE-MOLECULE AND COLLECTIVE DYNAMICS.

Research completed this year provides insights into the structure and dynamics of molecular liquid and complex fluid systems (e.g., nanoparticle and colloidal dispersions) where interfaces are known to play an important role. In one study, we used molecular simulations to investigate how the strength and the range of adsorbate-adsorbate and adsorbate-adsorbent attractions impact the thermodynamic and dynamic properties of fluids adsorbed in nanoporous materials. The results establish quantitative correlations between adsorption and diffusivity. In related work, we presented simulation data that demonstrate correlations between position-dependent density and diffusivity, respectively, in confined fluids. In our efforts to understand how interactions affect assembly using computer simulation, we discovered that fluids of particles with moderate size-polydispersity favor the formation of topologically close-packed Laves phases and related quasicrystalline structures at high density. We also demonstrated, in a related paper, how one can use inverse methods of statistical mechanics to design interparticle interactions that favor such phases in one-component systems. In the area of inverse design, we published new results on the assembly of porous single- and multicomponent assemblies using machine learning strategies.

Experimentally, we completed a study that demonstrated how the balance of repulsive and attractive forces can be tuned in a system of glutathione-coated gold nanoparticles in aqueous solution to reversibly form nanoclusters of a prescribed size by varying pH. Finally, we completed two investigations exploring how effective interactions between proteins in concentrated solutions can be tuned via the addition of cosolutes to reduce the shear viscosity.

FRANCIS T.F. TSAI, Q-1530, Baylor College of Medicine. STRUCTURAL AND MECHANISTIC STUDIES OF ATP-DRIVEN PROTEIN MACHINES.

Hsp104 is a ring-forming ATPase that cooperates with Hsp70 and Hsp40 chaperones to rescue stress- damaged proteins from both amorphous and amyloid-forming aggregates. The ability to recover functional protein relies upon pore loops present in the nucleotide-binding domain (NBD) of Hsp104 (loop-1 and loop-2 in NBD1, and loop-3 in NBD2), which face the protein translocating channel and couple ATP-driven changes in pore loop conformation to substrate translocation. A hallmark of loop-1 and loop-3 is an invariable and mutational sensitive aromatic amino acid (Tyr257 and Tyr662) involved in substrate binding. However, the role of other conserved aliphatic residues (Lys256, Lys258, and Val663), and the function of loop-2 in protein disaggregation has not been investigated. We recently determined a new crystal structure of an Hsp104 fragment, which crystallized in a different space group with three molecules in the asymmetric unit. Notably, Hsp104(1-360) exhibits molecular interactions involving loop-1 and loop-2, which resemble contacts with bound substrate. Corroborated by biochemical experiments and functional studies in yeast, we demonstrate that aliphatic residues flanking Tyr257 and Tyr662 are equally important for substrate interaction and abolish Hsp104 function when mutated to glycine. Unexpectedly, we find that loop-2 is sensitive to aspartate substitutions that impair Hsp104 function and abolish protein disaggregation when loop-2 is replaced by four aspartate residues. Our observations suggest that Hsp104 pore loops are mechanistically distinct and have non-overlapping functions with loop-1 facilitating protein binding, loop-2 potentially promoting protein unfolding, and loop-3 mediating substrate translocation through the Hsp104 hexamer.

BENJAMIN P. TU, I-1797, The University of Texas Southwestern Medical Center. SELECTIVE REGULATION OF METABOLISM BY A CONSERVED INHIBITOR OF TORC1.

Over the past year we have made significant progress on this project. We continued to dissect phenotypes of cells lacking the GATOR1 complex in both yeast and mammalian cells. Since NPRL2 KO embryos are unable to be born, we proceeded to conditionally delete NPRL2 (a component of the GATOR1 complex) in skeletal muscle, a highly metabolically active tissue, and determined the resulting phenotypes. Loss of NPRL2 in muscle causes constitutive activation of mTORC1 signaling and impairs fasting-induced autophagy in vivo. Muscle fibres of NPRL2 mKO animals are significantly larger and show altered fibre-type composition, with more fast-twitch glycolytic and less slow-twitch oxidative fibres. Consistent with this phenotype, NPRL2

muscle knockout mice have increased running behavior and enhanced glucose utilization. We observed that glucose flux into the TCA cycle is impaired by the loss of NPRL2, and the muscle exhibits an extreme Warburg metabolism with many hallmarks of aerobic glycolysis, including increased GLUT1 and LDH expression and phosphorylation of the pyruvate dehydrogenase complex. Remarkably, this switch in metabolic phenotype is entirely consistent with the phenotypes of *npr2* yeast cells, revealing that activation of TORC1 promotes a bona fide Warburg metabolism because key TCA cycle intermediates (i.e., oxaloacetate and 2-ketoglutarate) are consumed for making nitrogen-containing amino acids (i.e., aspartate and glutamine). The consumption of these TCA cycle intermediates necessitates an upregulation of glycolysis and lactate production for ATP and the regeneration of NAD⁺.

ADAM R. URBACH, W-1640, Trinity University. MULTIVALENT CUCURBIT[N]URILS FOR HIGH-AFFINITY REVERSIBLE BINDING.

1. A manuscript was recently submitted as a full article to JACS describing the first example of the molecular recognition of methionine-terminated peptides and non-aromatic peptides with submicromolar affinity in aqueous solution. The discovery was made from a focused library screen and confirmed by isothermal titration calorimetry (ITC). Due to the potential importance of this work for targeting unprocessed eukaryotic proteins, for which methionine is the N-terminal residue, we completed an in-depth investigation of the sequence-determinants required for high-affinity binding in this motif using a combination of ITC, electrospray ionization mass spectrometry, and NMR spectroscopy on 25 purified peptides.

2. A review was published as a book chapter for the Royal Society of Chemistry describing our work at the forefront of the molecular recognition of peptides and proteins within the broader context of the field and with a special focus on the importance of aromatic interactions in synthetic and biological protein complexes.

3. We are making slow but sure progress on the synthesis of cucurbit[n]uril-modified hydrogels for the purpose of studying multivalent binding. Monofunctional cucurbit[8]uril has only recently become available from our collaborator, and we have a gram of the material in house. The material is only weakly soluble in aqueous solution and insoluble in organic. We have developed a method to dissolve this material in DMSO as a PF₆ salt of a cationic guest complex. This sets the stage for the synthesis of a broad range of cucurbit[8]uril derivatives, for which the literature has no precedent.

KOSAKU UYEDA, I-1720, The University of Texas Southwestern Medical Center. BIOCHEMICAL MECHANISM OF THE GLUCOSE SENSING AND REGULATION OF ChREBP.

ChREBP dependent gene transcription is controlled by trafficking of ChREBP between cytosol and nucleus and altered efficiency of ChREBP binding to specific carbohydrate response elements in the genes. Nuclear export as well as import of ChREBP are regulated not only by the phosphorylation status but also by the interaction of ChREBP with 14-3-3 proteins and importin alpha. We have shown that the interaction between 14-3-3 and ChREBP not only promotes export of ChREBP from nucleus to cytosol under starved conditions and at the same time inhibits the import by blocking importin a binding to NLS site. Under high glucose ChREBP is imported into nucleus by binding to importin a and start transcription of the enzyme genes to activate lipogenesis. We have now solved the 3D structure of the ChREBP-NLS site complex, which shows major and minor binding domains, similar to known structures of NLS bound proteins. We found that interaction between importin alpha and NLS site peptide could be measured by fluorescence polarization (FP) and ITC measurements. In order to discover drugs to control obesity, we performed HT screening of a small library and found two potential inhibitors with IC₅₀ of less than 1 μM. Those compounds also inhibit the nuclear localization and transcription activities. We are currently collaborating with Dr Jef Debrabander in this department to synthesize more related compounds to improve the potency which ultimately leads to useful drugs. We will continue to investigate the biochemical mechanism how these compounds inhibit the interaction between ChREBP/importin a interaction leading to inhibition of fat synthesis.

RAFAEL VERDUZCO, C-1888, Rice University. CHARGE SEPARATION IN WELL-DEFINED DONOR-ACCEPTOR BLOCK COPOLYMER INTERFACES.

We completed an experimental and computational study of charge separation in model block copolymer systems. The block copolymers were comprised of conjugated donor and acceptor polymeric blocks linked by a flexible, non-conjugated linker. By systematically varying the length of the insulating linker group, we hypothesized we could tune the rates of charge separation and recombination at the donor-acceptor interface. Experiments revealed that the flexible linker significantly decreased rates of charge separation and recombination, and computational studies indicated this was primarily due to rotation of the conjugated polymers at the interface to a non-planar relative orientation of the blocks. This work demonstrated the impact that small structural changes at the interface can have on charge separation and suggests that a linker which prevents rotation of the donor and acceptor polymer blocks would be ideal for increasing the relative rate of charge separation.

We explored a new concept for mechanically robust and electronically active materials. Specifically, we incorporated a supporting elastic network in a bulk heterojunction donor-acceptor blend. Our method for incorporating the elastic network involved blending reactive small molecules with donor and acceptor semiconductors. The reactive molecules were crosslinked through either the thiol Michael addition or radical thiol-ene coupling reactions without disrupting the blend microstructure. This technique enabled us to incorporate up to 20 wt % thiol-ene network without any loss of functionality in the donor-acceptor blend. This work points to a new concept for producing robust and versatile organic semiconductor blends.

In related work, we developed shape-responsive polymer networks that could be programmed to reversibly transform between two arbitrary, non planar shapes. We studied structural changes in hybrid perovskite materials and the swelling behavior of surface attached polymer networks.

ERIC J. WAGNER, H-1889, The University of Texas Medical Branch. Cryo-EM ANALYSIS OF THE INTEGRATOR COMPLEX.

Overall Summary: During the three-year period of the Welch Grant support, my laboratory has published sixteen manuscripts and we have another four that are submitted. Of these 20 manuscripts, nine can be directly attributed to support from the Welch Foundation and the seven that are in press have acknowledged these vital resources. We are pleased to report that two of these publications connected to Welch support have been published in Year 3. Importantly, we note that two additional manuscripts that deal with the Integrator Complex (the focus of the Welch supported research) have been reviewed positively at both Science and Nature. In light of this productivity and exciting new findings, the Welch Foundation has renewed our grant support for another three years. Below are a few highlights of our work published or submitted in year 3.

- We have now determined that INTS4 binds to the INTS9/11 heterodimer and that manuscript is currently published at NAR. We have now expressed all three of these subunits as recombinant proteins and we are currently using EM to solve the structure of the heterotrimer. This is the subject of SA1 of the renewed grant.

-We have completed an extensive collaboration with several labs to show that Integrator performs an important function in the genome-wide attenuation of RNAPII in Drosophila cells. This work has now been reviewed at Science and we believe we have a strong chance of getting a revision accepted. This work has uncovered a fundamental function for Integrator.

-We have a collaborative manuscript that is currently under revision at Nature describing how the Integrator subunit 3 gene is a major target for deregulation in leukemia. This work is ground breaking as it will directly implicate compromise of Integrator function in cancer, which has not been described.

-We show that PP2A associates with Integrator and can dephosphorylated RNAPII CTD. This is the focus of SA2 of the renewed Welch grant.

YIHONG WAN, I-1751, The University of Texas Southwestern Medical Center. BIOCHEMICAL CHARACTERIZATION OF HOW MATERNAL MILK IMPACTS OFFSPRING EPIGENOME AND METABOLISM.

Our overarching theme is that milk quality significantly impacts the health of the offspring by not only regulating their postnatal development but also influencing their propensity to develop chronic metabolic disorders. We hypothesize that early postnatal exposure to inflammatory insults due to maternal milk defects may change the epigenetic landscape of the developing offspring, leading to metabolic abnormalities. In the second year of this funding period, we have made significant progress in all three Aims.

Aim 1: Our results reveal that WT pups nursed by VLDLR-KO moms display elevated inflammatory markers in fat compared with WT pups nursed by WT moms, which persists until early adulthood at 3 months old. We have performed detailed analysis on body weight and glucose metabolism in the offspring under chow or high-fat diet. We found interesting sex-dependent effects, in which only female offspring develop glucose intolerance upon high-fat-diet feeding whereas male offspring is less affected. We are currently examining in detail whether this glucose intolerance is due to reduced insulin production, insulin sensitivity and/or hepatic glucose production.

Aim 2: We have examined several epigenetic markers and histone modifications in the promoter regions of key inflammatory and metabolic genes in the fat of WT pups nursed by VLDLR-KO vs. WT moms. Moreover, we found that mTOR signaling and the synthesis of cholesterol precursors are elevated in the lactating mammary glands of VLDLR-KO moms compared with WT moms.

Aim 3: To explore pharmacological intervention, we are currently testing whether TLR4 inhibitor treatment in the pups not only prevents the inflammation but also the glucose intolerance caused by the milk from VLDLR-KO moms.

In summary, our progress during year 2 has met and exceeded the proposed goals. Our continued research will reveal more exciting findings on how maternal lactation defects impact offspring metabolism and disease propensity.

MENG C. WANG, Q-1912, Baylor College of Medicine. CHEMICAL IMAGING OF GLUTATHIONE SPATIOTEMPORAL DYNAMICS DURING AGING.

1.1 We introduced a cyano group to the Michael acceptor to increase the reaction kinetics and replaced the ketone with an amide to balance the equilibrium constant of the Michael addition in the mM range. Based on this design, we developed RealThiol (RT) that enables quantitative real-time imaging of GSH in living cells. This work has been published in Nature Communications 2017. 1.2. Based on the GSH probe design, we further introduced triphenylphosphium (TPP) to the probe to develop mitochondria-specific GSH probes, namely mitoRT. This work has been published in ACS Sensors 2017. 1.3. We developed organelle-specific GSH probes, HaloRT, and demonstrated nucleus-, cytosol-, and ER-specific GSH imaging. This manuscript is ready to be submitted in the next a couple of weeks. 2.1. In the preliminary study, we discovered that pyronines can reversibly react with H₂S. However, the equilibrium constant is in the 100 μM range. We tried to optimize the chemical structures to lower the equilibrium constants to the nM range. We also modified the 4-OH group of E2 with an azide group, which releases estrogen in the presence of H₂S, thus triggering enzymatic production of luminescence, and is working to increase the reaction speed between azide and H₂S. 3.1. 3.1. We are developing techniques to deliver the GSH probe and/or redox biosensors into the tissues. First, we have generated rAAV9 virus carrying mito-roGFP1 and delivered it into the mouse heart/liver by tail vein injection. Adult cardiomyocytes were isolated and imaged for expression of biosensor genes two weeks after injection and isolated cardiomyocytes were imaged for mitochondrial ROS in myocytes. Second, we are also developing an intraductal injection technique to deliver the GSH probe or redox biosensors into the mouse mammary gland and measure GSH/ROS levels.

QINGHUA WANG, Q-1826, Baylor College of Medicine. CHEMICAL MECHANISMS OF MUSCLE CONTRACTION AND REGULATION.

As the basic units of muscle contraction, sarcomeres are composed of thin filaments formed by actin, tropomyosin and troponin and thick filaments formed by myosin. Chemically, the interaction between actin and myosin and its regulation by tropomyosin and troponin constitute the foundation for muscle contraction. However, in the absence of high-resolution structures of these complexes, the chemical mechanisms of how ATP and its hydrolysis modulate the affinity between actin and myosin and whether tropomyosin regulates myosin binding to actin through a steric or allosteric mechanisms remain poorly understood. We have made excellent progress towards understanding the chemical mechanisms of these processes in the past year. We have successfully assembled the actin-myosin and actin-myosin-tropomyosin complexes in different nucleotide-bound states, and are currently employing single-particle cryo-electron microscopy and 3-dimensional reconstruction to obtain atomic structures of these important complexes.

YINGFEI WANG, I-1939, The University of Texas Southwestern Medical Center. BIOCHEMICAL CHARACTERIZATION OF PAAN.

Major accomplishment:

Recently, we identified a novel Poly(ADP-ribose) polymerase-1 (PARP-1) associated nuclease (PAAN) which has 3' exonuclease activity (Wang et al., Science, 2016). Detailed accomplishments during year 1 was summarized as following:

1) We have studied the importance of Y shape DNA structure, which mimics the intermediate status of DNA replication, as PAAN's 3' exonuclease activity substrates and further characterized PAAN's 3' exonuclease specificity in response to the different length of unpaired DNA at 3' end. Our data showed that PAAN prefer to recognize Y shape DNA substrates and cleave the short unpaired nucleotides at the 3' end, indicating that PAAN is likely to play a role in DNA replication.

2) We performed an in vitro elongation assay to confirm if PAAN removes misincorporated DNA at the 3' end and ensures the success of the elongation. Our data showed that PAAN has the proofreading function and coordinates with DNA polymerases without exonuclease activity to ensure the accuracy of the elongation process.

3) We knocked out PAAN in different cancer cells including MDA-MB-231 breast cancer and LN229 glioblastoma. We found that loss of PAAN significantly reduced DNA synthesis, inhibited colony formation under hypoxia conditions and attenuated the growth of breast tumor and glioblastoma in mice. Our results indicate that PAAN has DNA proofreading function and plays an essential role in DNA replication and tumor growth.

4) We also studied the role of hypoxia inducible factor (HIF) biological functions and epigenetic regulation.

5) Year 1 progress has resulted in 3 publications on respectful journals, including Nucleic Acids Res, J Clin Invest., and Cell Mol Life Sci.

6) Year 1 progress has also resulted in 6 invited talks at the international meeting and Universities.

Plan:

We will further study the role PAAN nuclease activity in DNA replication and tumor growth in vivo and investigate its underlying regulatory mechanisms.

YUHONG WANG, E-1721, University of Houston. THE KINETICS AND CONFORMATIONAL CHANGES DURING THE PEPTIDYL TRANSFERASE REACTION IN SINGLE RIBOSOMES.

We have developed super-resolution force spectroscopy (SURFS) with 0.5 pN force resolution, and revealed that the ribosome moves by half a nucleotide (breaking of one-H bond) upon the formation of the pre-translocation complex, which is beyond the resolution of other techniques. Some antibiotics mechanism were revealed. 2. We have developed a force-induced visualization method that can determine the functional positions of nucleic acids with single-nucleotide resolution. Further improvement was implemented since last year's report. The use of an adjustable mechanical force overcomes the variations of buffer conditions and analyte concentrations. We have demonstrated the application via probing the mRNA movement during ribosomal translocation, and revealing the interacting sites and strengths of DNA-binding drugs. Experimental recording and quantification can be achieved with a cheap and portable device coupled with a smart phone. Multiplexed detection can be realized by using acoustic radiation force. 3. The mRNA's precise 3-nucleotide movement is critical for translation fidelity. However, none of the current methods can reveal the mRNA dynamics near the ribosome entry site, which inhibits the understanding on this important issue. We have developed a dual DNA ruler toe-printing assay that provided such capability. By uniquely probing both the 3'- and 5'-termini of mRNA, we observed an antibiotics-trapped intermediate state in which the mRNA formed a looping state inside the ribosome by one nucleotide. This state is a direct evidence to suggest the ribosomal "inchworm" translocation mechanism. In addition, it is probably a high-energy state that precedes full translocation because complete translocation was observed after antibiotics wash-away. The same "looped" intermediate state persists on a "-1" frameshifting motif, indicating that frameshifting occurs afterwards.

ZHIGAO WANG, I-1827, The University of Texas Southwestern Medical Center. REGULATION OF NECROPTOSIS BY CASEIN KINASE 1.

Previously, we have shown that Casein Kinase 1 (CK1) family members alpha, delta, and epsilon are all recruited to the necrosome after necroptosis induction, through directly binding to RIPK3. We also demonstrated that all three CK1 kinases are able to phosphorylate S227 of RIPK3 in vitro. However, the functional importance of this interaction and phosphorylation were not addressed. During the past year, we made CK1-alpha, CK1-delta, and CK1-epsilon individual knockout cell lines, as well as a CK1-alpha/CK1-epsilon double knockout cell line. The double knockout line produced a much-reduced level of S227 phosphorylation of RIPK3 after necroptosis induction. It also showed much stronger resistance to cell death. In addition, knockdown CK1-delta in the double knockout cells further reduced RIPK3-S227 phosphorylation and cell death, suggesting that CK1 family proteins play redundant roles in phosphorylating RIPK3 to promote cell death. However, CK1 kinases are involved in many other cellular processes, notably cell cycle regulation, Wnt

signaling, and circadian regulation, which might influence cell death indirectly. To address this issue, we made point mutations in the RIPK3 protein that dramatically decreased the phosphorylation of S227 by CK1 kinases. This RIPK3 mutant also had much-reduced ability to activate necroptosis, again suggesting that phosphorylation of RIPK3 by CK1 kinases is important for necroptosis progression. Next, we want to develop a small peptide inhibitor that will block CK1 and RIPK3 interaction, hoping to use it in treating necroptosis-associated disease models. We believe the peptide inhibitor will block necroptosis without affecting other important CK1 functions, thus decreasing the off-target effect. We have narrowed down the smallest peptide in CK1-delta that is sufficient to interact with RIPK3 to only 18 amino acids. We are now in the process to make cell-permeable CK1 peptides to test in cell death assay.

CORAN WATANABE, A-1828, Texas A&M University. **STREPTOMYCES SAHACHIROI: A RICH TREASURE TROVE OF UNIQUE BIOSYNTHETIC REACTIONS.**

The genes *aziA3* and *aziA6* are hypothesized to be involved in the construction of the azinomycin epoxide moiety. *AziA3* has the domain architecture of an amino acid ligase (AL) domain, a ketoreductase (KR) domain, and a peptidyl carrier protein (PCP) domain; the *aziA6* gene, a type II thioesterase domain, lies directly adjacent to the *aziA3* gene, which might suggest that this TE domain would be involved in releasing the bound product from the PCP domain of *AziA3*.

We have successfully synthesized several fluorescent molecule capture agents as well as a biotin based capture agent, which might facilitate the isolation and structural characterization of the natural product intermediate bound to the phosphopantetheine arm of the *AziA3* module. The approach finds precedence in protein ligation, which works well at very low concentrations of protein. As a proof of principle experiment, we have evaluated these thiol capture agents *in vitro* with the *AziB* polyketide synthase module. *AziB* displays 2-methylbenzoic acid bound to its phosphopantetheine arm. LC-MS and NMR confirmed this capture strategy was successful with *AziB*. We have also successfully generated an *aziA6* deletion strain. Two overexpression systems with *AziA3* and *AziA3* (with KR domain deleted) within the *aziA6* deletion strain have been produced. The capture strategy will be used to identify the product of the *AziA3* reaction using the *AziA3* overexpression/*aziA6* deletion strain. Preliminary data has been obtained by LC/MS and the product is suspected to be the epoxide unit but is under further analysis.

Work will follow with the *AziA3* (with KR domain deleted)/*aziA6* deletion strain to determine the intermediate formed.

Additionally, an 18O-experiment tracking the fate of molecular oxygen in azinomycin biosynthesis lends credence for the involvement of a monooxygenase in the formation of the epoxide unit (manuscript submitted).

LAUREN J. WEBB, F-1722, The University of Texas at Austin. **SMALL MOLECULE INTERACTIONS WITH PROTEIN ASSEMBLIES: "DRUGGING" THE PROTEIN-PROTEIN INTERFACE.**

Extensive progress towards these research objectives has been made during the last grant period, resulting in 3 publications and 3 manuscripts in preparation (including an invited review in *Ann. Rev. Phys. Chem.* that extensively discusses our Welch-funded work, although the journal formatting template did not include an Acknowledgements section):

1. Our experiments rely on vibrational spectroscopy of nitrile probes inserted into a protein, but there is controversy and confusion in the literature about interpreting nitrile spectra in these molecules. This past year, we published a comprehensive experimental and computational analysis of two conflicting effects on the vibrational absorption energy of nitriles within green fluorescent protein (GFP): 1) electrochromic effects based on the reaction field of nearby polarizable molecules; and 2) quantum mechanical effects from hydrogen bonding. Our recent publication in *J. Phys. Chem. B* provides specific experimental and computational tests that can be used by a wide variety of researchers to accurately interpret experiments that depend on nitrile spectroscopy.

2. Our work on electric fields in the interior of lipid bilayer membranes in collaboration with the laboratory of Ron Elber has continued to develop. We have discovered that the amino acid tryptophan partitions into a lipid bilayer membrane composed of phosphatidylcholine lipids. Moreover, the equilibrium extent of partitioning is significantly greater for positively charged tryptophan than negatively charged tryptophan. We will submit these results for publication soon.

3. We have significantly expanded a collaboration with the laboratory of Jennifer Brodbelt using a combination of vibrational spectroscopy and the Brodbelt laboratory's Welch-supported work in mass spectrometry to understand protein-protein interactions. We have submitted one manuscript for publication and have an additional one to be submitted soon.

R. BRUCE WEISMAN, C-0807, Rice University. **OPTICAL STUDIES OF NANOCARBONS.**

We have extended our recently developed method of variance spectroscopy to compute the third moments of fluorescence intensity distributions from nanoparticle samples. This skewness analysis measures individualization versus clustering even when only a single structural species is present. It is thus the most effective method for finding the aggregation state of sorted nanotube samples. In another advance in spectroscopic nanotube characterization, we devised a new way to interpret absorption spectra to isolate the contribution from individualized nanotubes and assign a numerical quality index to the sample. This method should be generally valuable for assessing and comparing nanotube dispersions. We have also continued to explore the rich interactions between nanotube structures and single-stranded DNA oligos. We find that ssDNA with a particular base sequence exhibits selective recognition for one enantiomer of (7,5) nanotubes compared to the other. These have identical structures except that one is a right-handed helix and the other is left-handed. Remarkably, our kinetic spectroscopy study shows that the displacement of the DNA coating by a conventional surfactant occurs 100 times faster for one nanotube enantiomer than the other. Further investigation of such selective affinities may enable structure-selective nanotube photochemistry and novel sorting methods. In collaboration with biomedical researchers, we reported a study that uses novel optical technology to detect and locate sub-nanogram quantities of carbon

nanotubes inside living mice. This method may eventually lead to new tools for noninvasive cancer detection. Our ongoing collaborative effort to develop a nanotube-based technology for non-contact strain sensing has achieved significant improvements by using a dual-layer coating structure in which the nanotube strain sensors are applied to the specimen surface separately from a polymeric top coat layer.

KENNETH D. WESTOVER, I-1829, The University of Texas Southwestern Medical Center. DEVELOPMENT OF COVALENT TAK1 INHIBITORS.

We contributed to the development of a new compound named Takinib, a potent and selective TAK1 inhibitor that induces apoptosis following TNF- α stimulation in cell models of rheumatoid arthritis and metastatic breast cancer. We demonstrated that Takinib is an inhibitor of autophosphorylated and non-phosphorylated TAK1 that binds within the ATP-binding pocket and inhibits by slowing down the rate-limiting step of TAK1 activation. Overall, Takinib is an attractive starting point for the development of inhibitors that sensitize cells to TNF- α -induced cell death, with general implications for cancer and autoimmune disease treatment.

ROBERT L. WHETTEN, AX-1857, The University of Texas at San Antonio. FUNDAMENTAL CHEMICAL RESEARCH ON LARGER MOLECULAR NOBLE-METAL CLUSTERS.

During this project year, we have achieved progress on several related fronts, as documented in the new publications and prepared manuscripts section. Analysis of nanoclusters is inherently difficult especially using mass spectrometry because of their stability, solubility, and variability of their charge states. The bio-functionality has progressed with the construction of the Ag₂₉ cluster with 12 lipolate ligands which demonstrated antibacterial and antifungal activity. An important aspect in terms of understanding these nanomaterials is to have a theoretical understanding of the role the structures of these nanoclusters play in terms of absorbing radiation and how this leads to their bio-functionality. Also, as per university goals, we have developed robust collaborations with other investigators (e.g. Dr. Stephan Bach) and personnel (e.g. Dr. David Black) and have utilized infrastructure (both computational, instrumental as well as the small molecule screening facilities at the South Texas Center for Emerging and Infectious Diseases (at UTSA)). The investigations have been a collaborative effort between many departments at UTSA and Universities around the world to enhance and maximize the impact and reach of this research.

CHRISTIAN P. WHITMAN, F-1334, The University of Texas at Austin. STRUCTURE FUNCTION RELATIONSHIPS IN ENZYMES.

The tautomerase superfamily (TSF) consists of more than 11,000 nonredundant sequences present throughout the biosphere. Characterized members have attracted attention because of the unusual and key catalytic role of an N-terminal proline. The few characterized members catalyze a diverse range of chemical reactions, but the full scale of their chemical capabilities and biological functions remains unknown. To gain new insight into TSF structure–function relationships, we performed a global analysis of similarities across the entire superfamily and computed a sequence-similarity network to guide classification into distinct subgroups. Our results indicated that TSF members are found in all domains of life, with most being present in bacteria. The eukaryotic members of the cis-3-chloroacrylic acid dehalogenase subgroup are limited to fungal species, while the macrophage-migration inhibitory factor subgroup has wide eukaryotic representation (including mammals). Unexpectedly, we found that 346 TSF sequences lack Pro-1, of which 85% are present in the malonate semialdehyde decarboxylase subgroup. The computed network also enabled identification of similarity paths, namely sequences that link functionally diverse subgroups and exhibit transitional structural features that may help explain reaction divergence. A structure-guided comparison of these linker proteins identified conserved transitions between them, and kinetic analysis paralleled these observations. Our results also suggest that contemporary TSF members may have evolved from a short 4-oxalocrotonate tautomerase-like ancestor, followed by gene duplication and fusion. Our new linker-guided strategy can be used to enrich discovery of sequence/structure/function transitions in other enzyme superfamilies.

C. GRANT WILSON, F-1830, The University of Texas at Austin. PROGRAMMED SELF-ASSEMBLY OF NANOSTRUCTURES.

Our efforts to establish patterning techniques that enable production of particles with dimensions below 10nm led to a study of directed self assembly of block co-polymers. Safe living anionic polymerization protocols were developed that enable synthesis of block copolymers with well controlled molecular weight and polydispersity. We learned to incorporate silicon into one of the blocks and thereby render that block stable to etching under oxidizing conditions. environments. This enables selectively etching of the all organic block to provide high aspect ratio, high resolution patterns.

Thin films of some block copolymers can be induced to self assemble with their lamellar morphology standing perpendicular to the substrate by annealing them on a neutral surface that does not favor wetting one block over the other. In order to stand up our silicon polymers they must be sandwiched between two neutral surfaces. A process that sandwiches the copolymers between two neutral surfaces required invention of new polymers that undergo marked changes in properties upon heating. We found a class of materials that work well for this purpose.

The size of the features that can be generated by self assembly of block copolymers depends on the length of the polymer and the extent to which the blocks tend to phase separate. As the blocks become less compatible, the length of the chain (and the size of the structures) can be reduced and still undergo phase separation. We have found silicon containing block copolymers and the requisite surface treatments that allow formation of oriented and aligned lines and spaces that are 5nm in width. These materials assemble into line-space structures that are 1/20th of the diameter of an influenza virus. With the help of generous collaborators we have successfully transferred these very small structures into organic and inorganic substrates and are now seeing the first evidence of directed self assembly with 4nm lines and spaces.

LON J. WILSON, C-0627, Rice University. CARBON NANOCAPSULES FOR ADVANCED THERANOSTIC APPLICATIONS.

Over the past few years, numerous nanotechnology-based drug delivery systems have been developed in an effort to maximize therapeutic effectiveness of conventional drug delivery, while limiting undesirable side effects. Among these, carbon nanotubes (CNTs) are of special interest as potential drug delivery agents due to their numerous unique and advantageous physical and chemical properties. Here, we show *in vivo* favorable biodistribution and enhanced therapeutic efficacy of cisplatin (CDDP) encapsulated within ultra-short single-walled carbon nanotube capsules (CDDP@US-tubes) using three different human breast cancer xenograft models. In general, the CDDP@US-tubes demonstrated greater efficacy in suppressing tumor growth than free CDDP in both MCF-7 cell line xenograft and BCM-4272 patient-derived xenograft (PDX) models. The CDDP@US-tubes also demonstrated a prolonged circulation time compared to free CDDP which enhanced permeability and retention (EPR) effects resulting in significantly more CDDP accumulation in tumors, as determined by platinum (Pt) analysis via inductively-coupled plasma mass spectrometry (ICP-MS).

JIANG WU, I-1940, The University of Texas Southwestern Medical Center. TUMOR SUPPRESSION FUNCTION OF Brg1/SMARCA4 IS DISRUPTED BY DCLK1-MEDIATED PHOSPHORYLATION.

Brg1/SMARCA4 is the catalytic subunit of the chromatin remodeling BAF complex, which can activate or repress gene expression and is frequently mutated in various cancers. We hypothesize that the tumor suppression function of Brg1 is impaired by Dclk1-mediated phosphorylation. In the last year, we are making steady progress towards understanding the function and the regulation of Brg1 phosphorylation.

Using rescue experiments with non-phospho (SA) and phosphomimic (SE) variants of Brg1, our study in neurons showed that the phosphorylation is required for the activation of neuronal target genes.

Interestingly, the phosphomimic Brg1 failed to repress several Brg1 target genes. It is intriguing to hypothesize that Brg1 phosphorylation may distinguish its activator versus repressor function. Currently, we are testing several candidate Brg1-interacting co-repressors to see whether the interaction is reduced by Brg1 phosphorylation. We have generated knockin mice which contain the SA and SE variants of Brg1. We will use these mice to study the molecular and biological functions of the phosphorylation event.

In collaboration with Dr. Ken Westover's lab in UTSW, we applied a new and more specific Dclk1 inhibitor and confirmed that Dclk1 is required for Brg1 phosphorylation in neurons. In addition, we showed that the phosphorylation is also CamkII-dependent. Currently, we are investigating whether CamkII and Dclk1 function in parallel or in sequence. We also plan to collaborate with the Westover lab to determine whether the oncogenic function of Dclk1 is through regulating Brg1 activities. In addition to the calcium signaling in neurons, we discovered that Brg1 phosphorylation could also be induced by the Sonic hedgehog (SHH) signaling. Since Brg1 also switches from a repressor to an activator in response to SHH signaling, the phosphorylation may be a general mechanism regulating Brg1 activities.

CHONG XIE, F-1941, The University of Texas at Austin. PROBING THE *IN VIVO* CHEMISTRY IN THE BEHAVING BRAIN.

The project period 17-18 is the first year of this Welch Grant, we have focused on technical preparations and developments for the proposed studies. We have made progress in the following fronts.

1. Nanoelectronic neural threads (NET) that mitigate chronic tissue response and interface instability: Conventional neural electrodes have been fabricated out of hard materials such as silicon and metals with elastic moduli exceeding those of neural tissues by many orders of magnitude. This severe mismatch in bending stiffness is generally believed to contribute to the instability of the tissue-electrode interface and chronic tissue damage such as continuous leakage of blood-brain barrier, neuronal death, and glial scar formation. All these effects compromise the fidelity of electrochemical measurements made by these conventional electrodes in brain, especially over chronic time scales. The ultra-flexible NETs, designed and fabricated in our group, overcome these challenges and realize chronically stable intracortical recording. In our pilot study and the grant period 17-18, we have fabricated NET electrodes for the proposed studies in probing *in vivo* chemistry in the brain.

2. *In vitro* and *In vivo* electrochemical characterization of NET electrodes. We performed cyclic voltammetry at 50 mV/s and electrochemical impedance spectroscopy over a frequency range of 1 Hz to 10⁵ Hz test in both *in vitro* (phosphate buffered saline) and *in vivo* (implanted in mouse brain) settings to characterize the electrochemical performance of the NET electrodes. These measurements also provide us with important baseline information for our subsequent calibration of the electrochemical sensing by these electrodes.

3. Longitudinal *in vivo* optical imaging in the NET implanted brain. As another modality we will use to probe the brain chemistry, we have also established a chronic *in vivo* platform that combines NET electrodes with longitudinal optical imaging in the same behaving brain.

JIAN XU, I-1942, The University of Texas Southwestern Medical Center. *IN SITU* ANALYSIS OF THE STRUCTURE-FUNCTION OF TRANSCRIPTIONAL ENHANCERS.

Biochemical isolation and analysis of the chromatin interactions regulating genomic function is a long-sought goal. During the past grant year, we developed a new system to unbiasedly identify endogenous genomic locus-regulating molecular interactions. The CAPTURE (CRISPR Affinity Purification *in situ* of Regulatory Elements) system contains the nuclease-deactivated biotin-tagged Cas9 protein and a single guide RNA (sgRNA). The programmable sgRNA serves to direct dCas9 to a target genomic sequence in mammalian cells. Upon *in vivo* biotinylation of the dCas9 protein, the native genomic locus-associated protein, DNA and RNA complexes are isolated by high affinity streptavidin purification, and analyzed by proteomics and high-throughput sequencing for study of genomic locus-regulating protein, RNA, and long-range DNA interactions, respectively. The vast majority of disease-associated variations reside within non-coding regulatory elements and exert effects through long-range regulation of gene expression. The unbiased analysis of native

genomic locus-templated hierarchical events enabled by the CAPTURE methods will help define the underlying regulatory principles, thus significantly advancing our mechanistic understanding of the genome and genetic variation in human diseases (Liu et al., Cell 170:1028-1043). In other studies, we discovered that a significant fraction of SEs are hierarchically organized, containing both hub and non-hub enhancers. Hub enhancers share similar histone marks with non-hub enhancers, but are distinctly associated with cohesin and CTCF binding sites and disease-associated genetic variants. Genetic ablation of hub enhancers results in profound defects in gene activation and local chromatin landscape. As such, hub enhancers are the major constituents responsible for super-enhancer functional and structural organization (Huang et al., 2018 Nature Communications 9:943).

BORIS I. YAKOBSON, C-1590, Rice University. SCIENCE OF NEARLY-1D MATERIALS: FROM NANOTUBES TO NANOWIRES AND GRAIN BOUNDARIES.

During the past year we have published a large-scale molecular dynamics study explaining an amazing efficiency of salt (NaCl) as promoter for synthesis of very broad “library” of 2D-materials. This study determined the qualitative change in the gas-intermediates and accordingly the reduction of reaction barriers, overall accelerating the synthetic reactions or even enabling the syntheses previously unknown (in collaboration with and led by experimental lab, NTU-Singapore).

Another important line of work was motivated by the experimental observations of specific catalytic processes, enabled by various nanostructures. Among them, examples of the ORR (oxygen reduction reaction) catalyzed by the single-atomic ruthenium sites on nitrogen-doped graphene; electroreduction of CO₂ to hydrocarbons and oxygenate, catalyzed by nitrogen-doped graphene quantum dots; and a detailed theory of the mechanisms of the ORR on B- and/or N-doped carbon nanomaterials with curvature and edge effects.

To achieve a formation of 1D-nanostructures one emerging approach is to utilize the spinodal decomposition of 2D-alloys. We have explored theoretically the details of formation enthalpies and atomic ordering, and further extended our model toward quaternary alloy, where formation of clean 1D-heterojunction is now demonstrated (submitted work).

Last but not least, we extend and deepen investigation of a novel material whose synthesis was predicted in our lab—2D boron also known as borophene. Its distinct metallic conductivity suggests possible support for 2D-plasmons. During past year we performed detailed computation of plasmon dispersion and low-damping conditions. Most recently, we discovered (collaboration with Northwestern U.) and explained the formation of 1D-linear “defects” whose ordering signifies formation of new phases- superlattices. This further demonstrate intriguing coupling of the lattice ordering with the charge modulation—charge density waves (CDW).

NAN YAN, I-1831, The University of Texas Southwestern Medical Center. A MONOGENIC IMMUNE DISORDER ASSOCIATED WITH OLIGOSACCHARYLTRANSFERASE DYSREGULATION.

During the previous funding year, we identified a bioactive glycan that activates innate immune response in chronic autoimmune diseases such as TREX1-fs-associated SLE. We have submitted a manuscript on our findings and it was favorably reviewed by Nature Communication. We are currently performing additional experiment for the revision.

Title: A bioactive mammalian disaccharide activates STING-TBK1-dependent immune response associated with chronic autoimmune disease

Abstract: Glycans from bacterial pathogens and fungi are well known pathogen-associated molecular patterns that are recognized by the host immunity. However, surprisingly little is known about whether and how mammalian self-glycan activates the host immune response, especially in the settings of chronic disease. Using biochemical fractionation and two-dimensional HPLC, we identified one such bioactive fOS specie, the disaccharide Man β 1-4GlcNAc, in mammalian cells undergoing chronic autoimmunity. We found that both monosaccharide residues and the 1-4 linkage are critical for micromolar bioactivity of this monomeric disaccharide. We also determined that Man β 1-4GlcNAc is produced by OST hydrolysis of lipid-linked oligosaccharides in the ER lumen, followed by ENGase and mannosidase processing in the cytosol and lysosomes. Furthermore, The disaccharide stimulates a broad immune profile including interferon-stimulated genes (ISGs) and chemokine genes that are TBK1-dependent and the ISGs also require STING. Together, our data identify Man β 1-4GlcNAc as novel innate immune modulator associated with chronic autoimmune diseases.

In follow up work related to this manuscript, we are trying to identify the receptor for this bioactive self- glycan using biochemical means. Besides the TREX1 disease, we also randomly selected 20 lines of that human SLE B cells and 10 lines of healthy controls, and we found that SLE cells also contain elevated levels of free glycans.

DING-SHYUE YANG, E-1860, University of Houston. ULTRAFAST ELECTRON CRYSTALLOGRAPHY AND FEMTOSECOND SPECTROSCOPY OF STRUCTURAL TRANSFORMATION DYNAMICS IN TRANSITION METAL SYSTEMS.

Using time-resolved ultrafast electron diffraction (UED) in the reflection geometry, the photoinduced phase transition of solid-supported ultrathin films of vanadium dioxide (VO₂) was investigated. In this study, we were able to examine for the first time the impact of structural strains caused by the supporting substrate on the transformation pathways of 10-nm-thick crystalline VO₂, which has not been explored in all of the previous UED and time-resolved x-ray diffraction studies conducted on bulk or bulk-like specimens. Following the energy input via photoexcitation, we observed an ultrafast release of the compressive strain of ultrathin VO₂ along the surface-normal direction, which is accompanied by faster motions of V-V dimers that are more complex than simple dilation or bond tilting. At longer times, a laser fluence multiple times higher than the thermodynamic enthalpy threshold is required for complete structural conversion, and for certain crystalline domains the structural transition is inhibited even on nanosecond times because of the surface stress. These

results signify a time-dependent energy distribution among various degrees of freedom (electronic, local bonding, and lattice) and the complexity of the phase transition of VO₂, where structural strain is a crucial factor to consider.

The ultrafast carrier dynamics and generation of coherent acoustic phonons (CAPs) in a semiconducting rare-earth monochalcogenide were reported for the first time, using two-color pump-probe reflectivity. Compared to the carrier relaxation processes and lifetimes of conventional semiconductors (e.g., II-VI cadmium-based ones with photovoltaic applications), in YbS the recombination of photoexcited electrons with holes in localized f orbitals is found to take place rapidly with a time constant of <500 fs. Such carrier annihilation indicates the ultrafast nature of valence restoration of ytterbium ions after femtosecond photoexcitation switching and before CAPs emerge.

JIN YE, I-1832, The University of Texas Southwestern Medical Center. **BIOCHEMICAL CHARACTERIZATION OF THE FATTY ACID-UAS DOMAIN INTERACTION.**

During the past year, we have determined that interaction between FAF1, an UAS domain-containing protein, with polyunsaturated fatty acids (PUFAs) prevents peroxidation of these FAs. Using cells cultured in vitro, we observed that cancer cells deficient in FAF1 are particularly sensitive to inhibitors of Gpx4, an enzyme removing toxic products of PUFA peroxidation. We are now confirming this observation through various in vivo systems. If true, these observations not only address the functional significance of interaction between FAF1 and PUFA, but also raise the possibility to treat cancers such as glioblastoma known to contain genomic deletion of FAF1 with Gpx4 inhibitors.

Based on our on-going study of the FFA-mediated signal transduction pathways, we published a review article updating this pathway, and a research article revealing the importance of this pathway in development of kidney cancers. Another two articles originating from this pathway have been submitted for publication.

DANNY L. YEAGER, A-0770, Texas A&M University. **SOME ACCURATE NEW COMPLEX SCALED MULTICONFIGURATIONAL METHODS FOR ELECTRON-ATOM/MOLECULE SCATTERING RESONANCES.**

Resonances in electron atom/molecule scattering and Auger processes are metastable continuum states of the electronic Hamiltonian. They play important roles in diverse processes involving electron transport and energy exchange between electronic and nuclear motions, vibrational excitation of molecules or molecular ions by electron impact, and dissociative attachment and recombination which are processes of great importance in the outer space, the higher atmosphere and plasmas and discharges. A mechanism for DNA damage by low-energy electrons has recently been suggested to involve these resonances. Through the method of complex scaling, these resonances may be investigated using bound state rather than scattering theory techniques.

We further apply the complex scaled multiconfigurational spin-tensor electron propagator method (CMCSTEP) for the theoretical determination of resonance parameters with electron-atom systems including open-shell and highly correlated (non-dynamical correlation) atoms and molecules. The multiconfigurational spin-tensor electron propagator method (MCSTEP) developed and implemented by Yeager and his coworkers for real space gives very accurate and reliable ionization potentials and electron affinities. CMCSTEP uses a complex scaled multiconfigurational self consistent field (CMCSCF) state as an initial state along with a dilated Hamiltonian where all of the electronic coordinates are scaled by a complex factor. CMCSTEP is designed for determining resonances. We also studied numerical Hartree self-consistent field calculations of an autoionization resonance parameters for a doubly excited 2s², 3s², and 4s² states of He atom with a complex absorbing potential and Floquet calculations for H₂⁺ photoionization.

HSIN-CHIH YEH, F-1833, The University of Texas at Austin. **NANOCLUSTER BEACONS FOR HIGH SPECIFIC DNA METHYLATION DETECTION.**

With the Welch support, we have published two research articles with our collaborators within this cycle: "A flow-proteomic platform for analyzing protein concentration (FAP): Proof of concept for quantification of PD-L1 protein in cells and tissues" in *Bioelectronics and Biosensors* (2018, 117, 97- 103) and "Syndecan-1 in mechanosensing of nanotopological cues in engineered materials" *Biomaterials* (2018, 155, 13-24). This year we attempted to diversify the sensor applications of our fluorescent nanomaterial probes in protein detection and mechanosensing. Besides, we are trying to use the state-of-the-art next-generation DNA sequencing platform (MiSeq from Illumina) to broadly scan the nucleobase composition and geometry space and search for specific DNA sequences that nucleate silver clusters with desired optical properties. By using the hyperspectral-TIRF imaging system built in our lab, we can rapidly acquire emission spectra of an exceptionally large number of cluster species synthesized from a DNA library of 10⁷. So far only hundreds of DNA strands were studied by DNA microarrays or multi-well plates. While we knew a number of interesting sequences (motifs) can effectively activate silver clusters or tune their emission color, we do not know the design rules of these sequences. This is clearly limited by the current ligand composition search space. To elucidate the design rules and to diversify the metal clusters for biosensing, it is absolutely necessary to have a massively parallel method to screen a large library of DNA sequences. To our best knowledge we are the only group using NGS platform for NanoCluster Beacon optimization. We expect to publish this pioneered method and the selection result in late 2018. This platform can be further extended for methylated DNA detection.

SHERRY J. YENNELLO, A-1266, Texas A&M University. **INVESTIGATING THE EQUATION-OF-STATE FOR A TWO-COMPONENT NUCLEAR SYSTEM.**

A nucleus is a Fermi liquid composed of two components, neutron and protons. When two nuclei collide there can be an exchange of nucleons (neutrons and/or protons) due to the difference in chemical potential. When the initial nuclei have different neutron fractions the exchange will drive the

reaction partners toward a common value of neutron fraction. The composition of fragments resulting from the nuclear collision can be used to measure the amount of equilibrium attained during the reaction.

We studied neutron-proton equilibration in heavy ion reactions around the Fermi energy using three independent probes of the equilibration: 1) The isoscaling parameter α ; 2) The $A=3$ isobaric yield ratio $Y(3H)/Y(3He)$; and 3) The neutron-proton composition of the quasiprojectile (N/Z_{qp}) as reconstructed with the 4 π detector NIMROD. The NIMROD array is a 4 π charged particle array that consists of 228 detector telescopes covering between 3.6° and 167° located inside of a neutron calorimeter. This complete coverage with NIMROD allows for the reconstruction of the fragmenting quasiprojectile so that the amount of equilibration can be measured.

Incomplete N-Z equilibration is observed. A clear dependence of the degree of equilibration on the collision violence (impact parameter) is seen. Equilibration is not necessarily seen when an observable reaches a value mid-way between two reference points; rather, equilibration is seen when the same observable measured in two reaction systems, which are spatial reflections of each other, reaches a common value. Given this observation, an appropriate method for calculating the degree of equilibration was developed. The degree of equilibration is calculated for each method, and reasonable agreement is observed. The values of NZ_{eq} presented in this work are consistent between the three different probes employed. Comparison of this measurement with theoretical models can help to constrain the parameters of the nuclear equation.

GUIHUA YU, F-1861, The University of Texas at Austin. PROBING THE CHARGE STORAGE MECHANISMS OF MOLECULARLY-ASSEMBLED TWO-DIMENSIONAL INORGANIC SOLIDS.

We are very grateful of the support from the Welch Foundation, which leads to many exciting research progress and results in total 11 refereed articles published in a number of prominent journals in the past grant year, including in JACS, Angew. Chem. Int. Ed., Nano Letters, ACS Nano, Chem, Advanced Materials, Advanced Energy Materials, Advanced Functional Materials, and Chemistry of Materials.

1. Inorganic 2D holey nanosheets synthesis and self-assembly: In the past grant year, we have made significant progress on developing self-assembly methodologies for novel 2D nanoarchitected materials including oxides, selenides, and phosphides, e.g. Ni-Co-A ($A = P, Se, O$) by a new sacrificial-template method. This new class of 2D holey nanomaterials with controlled untrathin thickness and tunable holey sizes, enable exceptional materials for exciting energy storage and/or electrocatalysis applications. A series of significant works have been published in JACS, Angew. Chem., Nano Lett., ACS Nano, and we are invited to write a significant review article for Adv. Energy Mater. We also developed a microwave-assisted solvent-dependent controlled synthesis of Facet-Controlled Synthesis of Single-Crystalline {010}-Oriented LiMPO₄ Nanosheets, which was published in Chem. Mater..

2. Charge storage and electrocatalytic properties in energy storage and electrocatalyst. We further made important progress towards better understanding of charge transport/storage as well as electrocatalyst properties of the above-mentioned novel 2D holey nanomaterials. Detailed electrochemical measurements (e.g. Li⁺/Na⁺ storage and catalytic properties for OER, or ORR or HER) of these nanomaterials have been carefully investigated, resulting in several high-impact journal papers published in JACS, Angew. Chem., Nano Lett., ACS Nano, Adv. Mater., and Adv. Funct. Mater.. Given our significant contributions to the field, we are invited to write a significant review article for Adv. Mater.

HONGTAO YU, I-1441, The University of Texas Southwestern Medical Center. BIOCHEMICAL AND STRUCTURAL ANALYSIS OF COHESIN AND ITS REGULATORS.

The ring-shaped cohesin complex topologically entraps chromosomes and regulates chromosome segregation, transcription, and DNA repair. The cohesin core consists of the SMC1-SMC3 heterodimeric ATPase, the kleisin subunit SCC1 that links the two ATPase heads, and the SCC1-bound adaptor protein STAG1 or STAG2. The SCC2-SCC4 complex loads cohesin onto chromosomes. Prior to DNA replication, cohesin bound to chromosomes is dynamic, and can be removed by the cohesin-releasing factor WAPL. DNA replication transforms cohesin rings dynamically associated with chromatin into the cohesive form to establish sister-chromatid cohesion. Here, we show that, in human cells, cohesin loading onto chromosomes during early S phase requires the replicative helicase MCM2-7 and the kinase DDK. Cohesin and its loader SCC2-SCC4 associate with DDK and phosphorylated MCM2-7. This binding does not require MCM2-7 activation by CDC45 and GINS, but its persistence on activated MCM2-7 requires fork-stabilizing replisome components. Inactivation of these replisome components impairs cohesin loading and causes interphase cohesion defects. Interfering with Okazaki fragment processing and nucleosome assembly does not impact cohesion. Therefore, MCM2-7-coupled cohesin loading promotes cohesion establishment, which occurs without Okazaki fragment maturation.

We propose that the cohesin-loader complex bound to MCM2-7 is mobilized upon helicase activation, transiently held by the replisome, and deposited behind the replication fork to encircle sister chromatids and establish cohesion. Our study thus establishes a coupling mechanism between sister-chromatid cohesion and DNA replication.

YONGHAO YU, I-1800 The University of Texas Southwestern Medical Center. TARGETING PARP1 FOR THE TREATMENT OF SMALL CELL LUNG CANCER.

We have made significant progress towards the abovementioned two specific aims. We recently developed an analog-sensitive approach that allows PARP-specific ADP-ribosylation of substrates (Gibson et al., Science, 2016). We have also characterized the function of specific PARylation sites on important signaling molecule, e.g., C/EBP β (Luo et al., Molecular Cell, 2017).

PARP1 plays a critical role in regulating many biological processes linked to cellular stress responses. Although DNA strand breaks are potent stimuli of PARP1 enzymatic activity, the context-dependent mechanism regulating PARP1 activation and signaling is poorly understood. We performed global

characterization of the PARP1-dependent, Asp/Glu-ADP-ribosylated proteome in a panel of cell lines originating from benign breast epithelial cells, as well as common subtypes of breast cancer. From these analyses, we identified 503 specific ADP-ribosylation sites on 322 proteins. Despite similar expression levels, PARP1 is differentially activated in these cell lines under genotoxic conditions, which generates signaling outputs with substantial heterogeneity. By comparing protein abundances and ADP-ribosylation levels, we could dissect cell-specific PARP1 targets that are driven by unique expression patterns versus cell-specific regulatory mechanisms of PARylation. Intriguingly, PARP1 modifies many proteins in a cell-specific manner, including those involved in transcriptional regulation, mRNA metabolism, and protein translation. From translational perspective, such PARylation signatures might be used to predict the response of a breast cancer patient to chemotherapeutic agents and PARP1 inhibitors. This paper has been published (Zhen et al., Cell Reports, 2017). After its publication, this study also received wide media coverage (e.g., <http://www.welch1.org/grants-programs/research-grants/yonghao-yu>).

ANVAR A. ZAKHIDOV, AT-1617, The University of Texas at Dallas. **PHOTOCHEMISTRY OF NANOIMPRINTED HYBRID PEROVSKITES FOR PHOTOVOLTAICS.**

During the report period we have created nanoimprinted optoelectronic devices, including photovoltaic solar cells devices (PV) and various novel types of light emitting devices (LED) with perovskite emitting layers. We extended our designed nanostructured solar cells of revolutionary hybrid perovskite to pioneering dual use electrochemical devices that are light emitting solar cells (LESC) based on organohalide perovskites that has a general ABX₃ structure with organic (A= CH₃NH₃), inorganic (B=Pb, X=I) part. We use our pioneering CNT sheets and yarns as charge collectors, that can be tuned by electrochemical ionic gating. This first year of this project we have concentrated on the fundamental studies of ions migration in dual use LESK devices upon photoexcitation by a process of photo polling. Main photochemical and photophysical processes in MAPbI₃: lead trihalide perovskite are analyzed in new type of LESK devices. LESK with PCBM and C60 transport layers have been created and we studied its operation upon ionic gating (paper in ACS Photonics). We also have created perovskite active nanoantennas with nanoparticles created by laser ablation (paper in Nano Letters). The metasurfaces of perovskites are created for enhanced photoluminescence by pioneering nanoimprinting (NIL) techniques, which significantly improves the morphology and crystallinity of perovskite films (papers in ASC Nano and Optics Letters). We further have achieved significant improvement of PV solar cells and LED performance by nanoimprinting and obtained significant results in this area, described below in detail (published in series of papers added to Profile). We also created tandems of tunable temperature white color LEDs, (published in Phys. Stat Sol.), Our review on "Halide-Perovskite Resonant Nanophotonics" has been accepted for publication in Advanced Optical Materials, summarizing our work on nanostructured systems, including solar cells with CNT interlayers, LEDs and microlasers.

CHENGCHENG ZHANG, I-1834, The University of Texas Southwestern Medical Center. **IDENTIFICATION OF POTENTIAL THERAPEUTIC COMPOUNDS FOR HEMATOPOIETIC REGULATION.**

We have made significant progress as planned.

In Aim 1, we demonstrated that the Arginase-inhibitory small molecule SA stimulates proliferation of hematopoietic stem cells. We started to test the hypothesis that an agent that can inhibit Arginase activity has activity to modulate immune-related disorders and control cancer development. We studied the effects of SA in a bone marrow failure model. SA boosts the recovery of hematopoiesis in bone marrow failure caused by chemotreatment and irradiation through inhibition of Arginase activity. We are testing whether Arginase inhibitors can efficiently delay tumor development in several mouse models. In Aim 2, we developed a number of SA small molecule derivatives and anti-Arginase monoclonal human antibodies and tested their abilities in inhibition of arginase activity. We did not identify a small molecule chemical with enhanced ability compared to SA. Importantly, we developed a number of anti-arginase antibodies. One of the anti-Arginase antibody showed efficacy in decreasing Arginase activity in vivo. In addition, we also identified another anti-Arginase antibody that can enhance Arginase activity in vivo. We are characterizing these antibodies in more assays. It is possible anti-Arginase human monoclonal antibodies may be utilized to modulate the activity of extracellular Arginase in vivo, which may regulate the activity of hematopoietic stem cells and immune system, as well as tumor development.

CHUN-LI ZHANG, I-1724, The University of Texas Southwestern Medical Center. **CHEMICAL REGULATION OF HUMAN MOTOR NEURONS.**

Amyotrophic lateral sclerosis (ALS) is an adult-onset motor neuron disease, for which no effective treatment exists. A disease-relevant cell model is essential for the identification and validation of potential therapeutics, since live motor neurons cannot be directly isolated from living human patients. My laboratory has pioneered a cell reprogramming method to generate functional motor neurons directly from fibroblasts of adult human patients. Our earlier work showed that these induced motor neurons (iMNs) can be used for modeling human ALS in a dish. Using this unique cell model, we conducted a screen of chemicals and identified a small molecule that is able to improve survival of human ALS-iMNs. Our ongoing work is focusing on understanding the molecular and cellular mechanisms by which the hit compound improves function of ALS-iMNs.

Since ALS is an adult-onset neurodegenerative disease, aging is a critical factor. A critical question is whether our human iMNs maintains aging-associated features. In the past funding period, we also systematically analyzed the aging status of iMNs from fibroblasts of human patients at different ages. In comparisons, we also obtained iPSCs from the same set of human fibroblasts and differentiated these iPSCs into motor neurons. Our analysis showed that skin fibroblasts exhibit aging-associated features, such as DNA damage, heterochromatin, nuclear envelope, and aging-associated beta-gal activity. The aging-associated features are maintained when these fibroblasts are directly reprogrammed into iMNs. In contrast, the aging-associated features are completely lost

in iPSCs and their derived motor neurons. Such a result indicates that iMNs rather than iPSCs-derived motor neurons are better suited for modeling adult onset ALS.

JUNJIE ZHANG, A-1863, Texas A&M University. FUNCTIONS OF UNIQUE STRUCTURES IN MYCOBACTERIUM TUBERCULOSIS TRANSLATION.

We have solved near-atomic structures of the Mtb 50S ribosomal subunit and the complete Mtb 70S ribosome by cryo-electron microscopy. We saw, upon joining of the large and small ribosomal subunits, a 100-nt long expansion segment of the Mtb 23S rRNA, named H54a or the 'handle', switches interactions from with rRNA helix H68 and rProtein uL2 to with rProtein bS6, forming a new intersubunit bridge 'B9'. In Mtb 70S, bridge B9 is mostly maintained, leading to correlated motions among the handle, the L1 stalk and the small subunit in the rotated and non-rotated states. We discovered two new protein densities near the decoding center and the peptidyl transferase center, respectively. These results provide a structural basis for studying translation in Mtb as well as developing new tuberculosis drugs.

RENYI ZHANG, A-1417, Texas A&M University. CHEMICAL KINETICS AND MECHANISM OF HYDROCARBON OXIDATION REACTIONS.

Experimental and theoretical studies have been carried out to investigate the hydrocarbon oxidation reactions initiated by the hydroxyl radical (OH) and ozone (O₃) and to assess their contributions to formation of tropospheric ozone and secondary organic aerosol (SOA). Progress has been made in experimental and theoretical studies of the oxidation of biogenic (isoprene and pinenes) and anthropogenic (toluene and xylene) hydrocarbons. A novel quasi-atmospheric aerosol evolution study (QUALITY) chamber, which consists of a bottom flow chamber through which ambient air is pulled continuously and an upper reaction chamber where aging of seed particles occurs, has been developed for monitoring of aerosol properties in the atmosphere. Our results indicate that initial photochemical aging of black carbon particles leads to considerable modifications to morphology and optical properties but does not appreciably alter the particle hygroscopicity under polluted environments. In addition, using combined theoretical and experimental methods, we show novel oligomer formation from methylglyoxal with the carbenium ions as the key intermediate. This cationic oligomerization is characterized by barrierless and irreversible pathways and occurs at fast rates in weakly acidic media, i.e., on fine aqueous aerosols and cloud/fog droplets under typical tropospheric conditions. Our results reveal that the carbenium ion-mediated reactions of -dicarbonyls provide the major sources for SOA and brown carbon formation and their importance is far larger than is currently recognized.

XUEWU ZHANG, I-1702, The University of Texas Southwestern Medical Center. STRUCTURAL AND FUNCTIONAL ANALYSIS OF THE BCCIP β /RPL23 COMPLEX.

We were able to form the complex between BCCIP β and RPL23, but it did not crystallize. In the past year, we have generated numerous constructs of both proteins, including deletions of flexible loops and terminal truncations in order to stabilize the complex for crystallization. We have successfully generated many modified RPL23 proteins that are more rigid and retain the binding to BCCIP β . These proteins will be subjected to co-crystallization. Meanwhile, the mutational analyses shed light onto the surface on RPL23 that may be involved the interaction with BCCIP β . Another strategy that we used was to design a linker to covalently link the two proteins. Moreover, EIF6 is another protein that interact with RPL23.

We are testing the formation of the BCCIP β /RPL23/EIF6 triple complex for crystallization. Function wise, we found that overexpression of BCCIP β in cells dramatically increase the levels of endogenous RPL23, supporting the idea that BCCIP β serves as a chaperone for RPL23. In the coming year, we will continue our efforts on crystallization and structural analyses of the BCCIP β /RPL23 and BCCIP β /RPL23/EIF6 complexes. In case crystals of the complexes are still difficult to obtain, we will use the crystal structures of the individual proteins to generate docking models, which will guide our design of point mutations in each protein to probe residues that are important for their interactions. Once key residues defined, we will test the effects of mutating these residues on the stabilization effect of RPL23 in cells.

YAN JESSIE ZHANG, F-1778, The University of Texas at Austin. VISUALIZATION OF THE INCORPORATION OF MOLECULAR OXYGEN IN ENDOPEROXIDE BOND FORMATION USING TIME-RESOLVED X-RAY CRYSTALLOGRAPHY.

Sulfur incorporation in the biosynthesis of ergothioneine, a histidine thiol-derivative, differs from other well-characterized transsulfurations. A combination of a mononuclear non-heme iron enzyme-catalyzed oxidative C-S bond formation and a subsequent pyridoxal 5'-phosphate (PLP)-mediated C-S lyase reaction leads to the net transfer of a sulfur atom from a cysteine to a histidine. In this study, we structurally and mechanistically characterized a PLP-dependent C-S lyase Egt2, which mediates the sulfoxide C-S bond cleavage in ergothioneine biosynthesis. A cation- π interaction between substrate and enzyme accounts for Egt2's preference of sulfoxide over thioether as a substrate. Using mutagenesis and structural biology, we captured three distinct states of the Egt2 C-S lyase reaction cycle, including a labile sulfenic intermediate captured in Egt2 crystals. Chemical trapping and high-resolution mass spectrometry were used to confirm the involvement of the sulfenic acid intermediate in Egt2 catalysis.

In addition, we have solved the structure of EgtB, an a-KG-dependent mononuclear non-heme iron enzymes that mediate the C-S bond formation in the second step of ergothioneine biosynthetic pathway. We understand the specificity of this enzyme through its complex structures with various substrates. In particular, two tyrosine molecules found at the active site have compensatory effect to mediate the nucleophilic reaction to mediate C-S bond formation.

JOHN C.-G. ZHAO, AX-1593, The University of Texas at San Antonio. EXPEDITIOUS MODIFICATION OF ORGANOCATALYST STRUCTURES FOR IMPROVED STEREOSELECTIVITIES.

In the past grant year, our Welch grant was reinstated in June 2017 and our lab was reopened subsequently. Since overall one year was lost due to the incident happened in 2016, in order to recover some of the losses, the first thing I did was to hire the all necessary personnel to restart the research as soon as possible. However, due to the slow visa process, it took them up to six months to arrive at UTSA. Despite the delay, we made excellent progresses on the proposed research in the past year. We have completed: 1) the revision of a manuscript on prolinal dithioacetals (submitted before the incident) and it is now published (Tetrahedron); 2) the synthesis of some new catalysts for the aldol reaction (submitted to Curr. Organocatal.); 3) the MDO-catalyzed anti-Mannich reaction (submitted to Tetrahedron); 4) the MDO-catalyzed synthesis of 3-oxabicyclo[3.3.1]nonan-2-ones (submitted to Adv. Syn. Catal.); 5) MDO-catalyzed diastereodivergent synthesis of tricyclic 2-chromanones (manuscript in preparation for Org. Lett.); and 6) MDO-catalyzed synthesis of 2-chromanones (manuscript in preparation for Org. Biomol. Chem.). There are several additional projects going very well right now in the lab and we expect to see some additional publications this year. In addition to the above, the two papers we submitted last year were officially published (Chin. Chem. Lett. and Mini-Rev. Org. Chem.). We also published a long review article on domino reaction (Adv. Synth. Catal.) that was chosen by the journal editor as a "Very Important Publication". Moreover, our collaboration with Professor Chen also come to fruition: We published three additional papers together last year (Chem. Commun.; Cryst. Growth Des.; and J. Solid State Chem.).

ALEXEY M. ZHELTIKOV, A-1801, Texas A&M University. OPTICAL DETECTION OF ULTRAFAST ELECTRON DYNAMICS AND SMALL-SCALE TEMPERATURE VARIATIONS IN CHEMICAL SYSTEMS.

The main accomplishments in the above-listed areas of research are as follows:

Quantitative fluorescence imaging of genetically encoded calcium sensors, indicating a calcium-ion influx through a cell membrane, has been combined with in situ single-cell fiber-optic quantum thermometry to enable an all-optical thermodynamic characterization of thermosensitive cell-membrane ion channels. In the method developed under this project, intensity of the calcium-sensor fluorescence is measured as a function of the cell temperature, which is read out by a specifically designed fiber-optic quantum thermometer, also developed as a part of this project. This method enables an accurate determination of the fundamental thermodynamic parameters of thermosensitive membrane ion channels, including entropy and enthalpy changes needed for heat-induced ion-channel gating. Based on this analysis, we have identified the parameter space within which laser thermogenetic neurostimulation can be confined to a single neuron and extended to deep brain regions.

Fluorescence imaging using fluorescent calcium sensors has been shown to provide a powerful tool for a quantitative characterization of single-cell laser thermogenetic neurostimulation. When combined with in situ quantum thermometry using NV centers in diamond integrated into an optical fiber, this approach enables a robust and reliable detection of thermogenetic stimulation of single neurons, helps discriminate between activated and silent neurons and provides a unique tool to measure complex patterns of neural activity modulated by finely tailored trains of laser pulses.

We developed a new all-optical method for time-resolved studies of ultrafast photoionization in complex chemical condensed-phase systems. Experimental and theoretical analysis of spectra of optical harmonics generated by ultrashort laser pulses has revealed important properties of ultrafast, multiple-pathway molecular dynamics in complex condensed-phase systems.

QING ZHONG, I-1864, The University of Texas Southwestern Medical Center. IDENTIFICATION OF AUTOPHAGY-SPECIFIC FACTORS FOR AUTOPHAGOSOME-LYSOSOME FUSION.

The HOPS complex has been shown to function as a tethering factor in yeast vacuole fusion through its interaction with yeast RAB7 YPT7. This protein complex is required for autophagy and it physically interacts with STX17. To investigate the role of HOPS in fusion, we have purified the human HOPS complex from human cells. Interestingly, in human cells, it is reported that HOPS doesn't interact with Rab7 directly. It is possible that other Rabs or Rab interacting proteins function in this process. Recently, Rab2a was reported to interact with HOPS directly and likely plays an important role in autophagy. We have identified a previously undescribed Rab that also interacts with HOPS and STX17, which is Rab39. In our preliminary experiments, Rab39 is important for autophagosome fusion with lysosome and directly interacts with HOPS. The interaction between HOPS and Rabs might complete their functions in autophagic fusion, which will be tested in biochemical and genetic assays.

We have identified more than 30 STX17 associated proteins by tandem affinity purification, and among them, at least 11 of them have shown at least partial colocalization with LC3 labeled autophagosomes. These potential autophagy regulators will be further validated in the following assays: 1). Endogenous colocalization assays. One of the candidate proteins, STXBP5, directly interacts with STX17, and its depletion in mammalian cells leads to autophagic fusion defect. Expression of GFP-tagged STXBP5 in stable cell lines revealed that it mainly localizes to autolysosomes/lysosomes. It also competes binding of SNASP29 to STX17. All of these data suggest that STXBP5 might be a critical regulator in autophagosome fusion with lysosomes. We will further explore its precise function and mechanism in this process.

YUBIN ZHOU, BE-1913, Texas A&M University Health Science Center. OPTICAL REWIRING OF EPIGENETIC LANDSCAPES TO REPROGRAM CELL FATE.

(a) Research Progress and Publications. During the second fiscal year, we have completed most of the experiments proposed in Aim 1 (to generate an inducible epigenetic remodeling toolkit) and also made steady progress and generated critical reagents that are essential for experiments in Aim 2 (to control epigenomes with optogenetic tools), with a total of 7 papers published in premier peer-reviewed journals that are directly related to the project, including

Angew Chem, Chem Sci, Nature Cell Biology and ACS Synthetic Biology (see Publications below). In addition, 4 manuscripts are under revision with reputational journals including Nature Chemical Biology, Cell Chemical Biology, PLOS Biology and Oncogene (accepted). Our optogenetics-related research has been prominently highlighted by NIH- NIGMS (<https://biobeat.nigms.nih.gov/2018/04/optogenetics-sparks-new-research-tools/>).

(b) Education. Dr. Lian He, sponsored by the Welch Foundation graduate fellowship and just graduated with a PhD degree, contributed to 10 publications. She was also the recipient of several poster or presentation awards from FASEB and Gordon research conference. Discoveries made from the Welch- funded project are also reported by media outlets (e.g., Photonics Media, BioTechniques, BioOptics World) to educate lay audience. The chemical biology toolkit tailored for gene regulation and cell signaling manipulation (as proposed in Aims 1 and 2) was also highlighted by JACS Spotlight, Royal Society of Chemistry, and featured as cover stories by Chemical Science and Angew Chem. One research product made during the fiscal year (CaRROT for transcriptional reprogramming; ACS Syn Biol '18) has been in the process of being licensed to a synthetic biology company (Refuge Bioscience Inc.) for translational applications.

All these efforts set the stage for evolution of LiSPIDER tools as proposed in Aim 1, and further applications to control the fate of mammalian cells (Aim 2) in Year 3.

CHAIR GRANTS

ZHIQIANG AN, CHAIR AU-0042, The University of Texas Health Science Center at Houston.

Dr. An's laboratory is well published and funded during the 2017-2018 academic year. The group currently consists of more than 15 students, postdoctoral fellows, and scientists. Dr. An authored/co- authored multiple peer reviewed scientific journal articles and presented scientific lectures in universities, industries, and at conferences both nationally and internationally during the 2017/2018 academic year. Dr. An lab is well funded by grants from CPRIT, DoD, NIH, and industry sources. Dr. An was also active in both graduate student and postdoctoral fellow training and in participation of committees and other professional activities, including journal editorial boards.

ERIC V. ANSLYN, CHAIR F-0046, The University of Texas at Austin.

Research in the Anslyn group is primarily focused on the creation of chemical sensors, novel supramolecular assemblies, and detailed mechanistic investigations. In the last year and since the prior report, we have published 7 papers that cite the Welch Regents Chair support (F-0046). With regards to chemical sensing, we developed a differential sensing array of peptide-appended fluorophores that were assembled on DNA double helices to classify and differentiate a wide variety of cell types associated with various cancers. The approach used chemometrics and showed that cells not part of the training set could be identified as such. We also created the first auto-inductive cascade for signal-amplification in the detection of thiols and showcased its utility in the quantification of the presence of VX nerve agent surrogates. With regards to supramolecular assembly, the group created a series of novel peptides with unnatural amino acids that could assemble into controlled loops, ladders, figure-eights, and linear polymers. Remarkably, when the assemblies were created from known antimicrobial peptides, the antibiotic activity was markedly enhanced. Further, we created a "click" reaction that assembles catechols with hydroxylamine spontaneously with the ability to label L-DOPA containing peptides and proteins. Lastly, with regards to physical organic studies, our group settled a very long-standing debate concerning the mechanism by which boronic-acid sugar sensors turn-on fluorescence upon binding saccharides. The photophysical studies revealed that the B-OH rotors of the boronic acids act as excited state energy acceptors by internal conversion, and upon conversion of these groups to boronate esters the "loose-bolt" internal conversion mechanism is arrested, thus allowing the emission quantum yield to increase. In summary, the Anslyn group made several fundamental scientific breakthroughs over the previous year by virtue of funding from the Welch Foundation.

DANIEL W. ARMSTRONG, CHAIR Y-0026, The University of Texas at Arlington.

First area of interconversion of three novel pentahelicene derivatives {3,5-bis (trifluoromethyl) benzo [i] pentahelicene, naphtha{1,2-i} pentahelicene and 4-methoxybenzo[i]pentahelicene as well as dive braryl atropisomera computer assisted deconvolution metho was employed to determine the individual peak areas and the retention times required for the calculation of apparent enantiomerization energy barriers, enthalpy and entropy of the interconversion of the pentahelicene derivative enantiomers. An ab initio quantum chemistry method was used to estimate theoretical kinetic and thermodynamic interconversion parameters and to evaluate the experimental data. For the atropisomers the racemization rates at different temperatures led to the value of the rotational energy barrier for racemization, and to the racemization half lifetime, $t_{1/2}$, indicating the atropisomer thermal stability. Second area these amines encompass a variety of structural and drug classes which are particularly important to the pharmaceutical industry and in forensics. Eighteen racemic controlled substances were simultaneously baseline separated in a single liquid chromatography-mass spectrometry (LC-MS) analysis. Second, E/Z tobacco-specific nitrosamines and their enantiomers were directly separated. The methodology of this study could be applied to cancer studies, and lead to more information about the role of these isomers in other diseases Third was compared to their linear counterparts, an increase in the kinematic viscosities and lower densities were observed. Thermal stability was found to be highly dependent on the position of the alkyl substituent group along with the length of the spacer chain. While the substitution on the alpha carbon of a spacer chain resulted in a significant decline in the thermal of DILs, the effect of mid-chain substitution on their stability was negligible.

VYTAS A. BANKAITIS, CHAIR BE-0017, Texas A&M University System Health Science Center.

Sec14-like PITPs integrate lipid metabolism with phosphoinositide production. We identified the first inhibitors of Sec14 and the 'bar-code' that governs drug sensitivity in Sec14-like proteins. We are engaged in total gene synthesis to define mechanisms of inhibition, and design of leads for next-generation anti-fungal drugs. Our description of a novel chemical scaffold for Sec14 inhibitors was published this year in CELL CHEMICAL BIOL.

We discovered a PITP pair supports development of the embryonic mammalian neocortex at the level of neural stem cells (NSCs). A paper describing those results, "A Golgi Lipid Signaling Pathway Controls Apical Golgi Distribution and Cell Polarity During Neurogenesis", was published this year in DEVELOPMENTAL CELL. With Hongyan Wang (Duke-NUS), we found a fly PITP regulates NSC homeostasis. That study, "Vibrator and PI4KIII Govern Neuroblast Polarity by Anchoring Non-muscle Myosin II", was published this year in eLife.

To understand how PITPs work, we must understand how these proteins bind/release their ligands. All-atom molecular dynamics simulations provide the first insights into the PITP lipid exchange cycle ("Dynamics and Energetics of the Mammalian Phosphatidylinositol Transfer Protein Phospholipid Exchange Cycle" published this year in the J. Biological Chem.).

Kes1 is a member of the functionally enigmatic, oxysterol binding protein-related protein (ORP) superfamily. We discovered Kes1, and other ORPs, are novel inhibitors of the G1/S cell-cycle transition, promote replicative aging, and that Kes1 is a major non-histone target for the NuA4 lysine acetyltransferase. Those results describing ORPs as novel integrators of lipid signaling with cell cycle progression (tumor-suppressors?) were published this year in DEVELOPMENTAL CELL ("The Kes1- Sec14 lipid signaling axis controls cell cycle and membrane trafficking systems").

ALLEN J. BARD, CHAIR F-0021, The University of Texas at Austin.

Over the reporting period (June 1, 2017 through May 31, 2018), we have extended the field of studying collisions on ultramicroelectrodes (UMEs) to the electrodeposition of an isolated platinum atom or small cluster, up to nine atoms, on a bismuth UME. The size and number of atoms of a cluster was predicted through electrochemical characterization. This new methodology permits the atom-by-atom fabrication of isolated platinum deposits, ranging from single atoms to 9-atom clusters. Using a collision approach, we have also developed ultrasensitive electro-analysis which was demonstrated with femtomolar determination of lead, cobalt, and nickel. We also developed ultra-sensitive potentiometric measurement of dilute redox molecule solutions and determined sensitivity factors at platinum UMEs.

We have continued pursuing investigations with scanning electrochemical microscopy (SECM) by determining mechanisms of important reactions including in situ detection of the adsorbed iron (III) intermediate and mechanism of magnetite electrodeposition, and the detection of the carbon dioxide radical in the electrochemical reduction of carbon dioxide in N, N-dimethylformamide. These studies involved the use of scanning electrochemical microscopy at the nanometer level. We have also maintained our interest in the surface interrogation mode of SECM, which has been used to study catalysts and attain information on intermediates during electrocatalytic reactions. For example, we have tested one of the most active transition metal phosphides, cobalt phosphide, for its stability and operability under mild conditions that it may be exposed to in its applications (i.e., photo-electrochemistry and artificial photosynthesis). We also investigated the photoactivities of lead chromates with various combinations of lead and chromium using the rapid screening mode of SECM.

ANDREW R. BARRON, CHAIR C-0002, Rice University.

Electrical measurement on individual CNTs shows a distance relationship opposite of what expected for conductor. This is found to be due surface contamination. Removal of which shows resistance length relationship. But at small probe distances still have a high resistance due to the creation of depletion zones under the junction. These depletion regions are also observed where 2 CNTs cross. The magnitude of the resistance is dependent on the resistance at junction $\propto 1/\text{difference in diameter of CNTs}$. Where this junction resistance is high, passing a high voltage through one of the CNTs causes it to break at the junction of the two CNTs. This results in 2 halves of an original CNT that can be physically manipulated to make an experimental (rather than computational) measurement for 1st time of the resistance between 2 CNTs that are 100% guaranteed to be the same chirality and diameter. In doing so it is found that there exists an angular dependence of the CNT-CNT junction resistance that is maximized at 30° and minimized at 45°. It is also possible to confirm for the 1st time that there exists a sinusoidal relationship between the resistance of 2 parallel CNTs as a function of their overlap length. Measurements with W, Cu, Au, and Cr probes demonstrates that the M-CNT resistance is lowest for Cu and computation shows this is related to an increase in new states around the Fermi energy that enhance the conductivity of Cu. Impact: 1) nano devices may have a limit of how nano they can be due to junction depletion zones; 2) for maximum conductivity of CNT fibers the diameter of the CNTs must be as mono-dispersed as possible; 3) CNT-CNT conduction is related to microwave waveguide coupling; 4) the presence of nano carbon increases the conductivity of Cu by new states around the Fermi level.

RAY H. BAUGHMAN, CHAIR AT-0029, The University of Texas at Dallas.

Welch Chair support helped enable 6 refereed publications in archival journal, including publications in Science, in a Nature journal, and in the Proceedings of the National Academy of Science. This funding also helped enable the issuance of six US patents (and many more foreign patents), all of which have been licensed to a company that is creating jobs in Texas (Lintec). The Welch Chair supported NanoExplorer high school students (about 35 strong in the program year), our undergraduate students, and our outreach events for students of all ages. Welch Chair seed funding was leveraged to obtain NanoTech Institute funding from the United States Air Force, the United States Navy, the United States Army, and the NSF. In the above mentioned publication in Science, we report carbon nanotube yarn harvesters that electrochemically convert tensile or torsional mechanical energy into electrical energy, without requiring an external bias voltage. For the important frequency range between a few Hertz and 30 Hz, no other mechanical energy harvester can generate a

higher output electrical power. These energy harvesters were used in the ocean to harvest wave energy, combined with thermally-driven artificial muscles to convert temperature fluctuations to electrical energy, sewn into textiles for use as self-powered respiration sensors, and used to power a LED and to charge a storage capacitor. In the article in the Proceedings of the National Academy of Sciences (whose image is on the journal cover), we reported an inexpensive method to fabricate graphene sheets that are nearly as strong as the carbon fiber polymer composites used for aircraft, and able to absorb much greater energy in all in-plane directions before failing.

TADHG P. BEGLEY, CHAIR A-0034, Texas A&M University.

1) Radical SAM enzymes: For MqnE (menaquinone biosynthesis), we have completed the synthesis of a mono-deuterated substrate analog to analyze the active site conformation of the initially generated captodative radical by EPR. We have also completed our characterization of the inhibition of MqnE by a substrate analog that adds to the adenosyl radical and then abstracts a hydrogen atom from the enzyme to give a bisubstrate inhibitor ($K_i = 3$ micromolar and IC_{50} of 1.8 micromolar and 13.6 micromolar against *H. pylori* and *C. jejuni* respectively). We have successfully reconstituted the MqnC-catalyzed reaction (next step in menaquinone biosynthesis) using a designed substrate to increase the product yield substantially. It is now possible for us to carry out mechanistic studies on MqnC and we have also successfully trapped an aryl radical anion intermediate. The improved reconstitution also gives us access to sufficient quantities of the MqnC reaction product that we can initiate mechanistic studies on the next enzyme on the pathway (MqnD).

For HBI synthase (paralog of the thiamin pyrimidine synthase), we have completed the EPR characterization of an early radical intermediate. To understand the complex reaction catalyzed by the bacterial thiamin pyrimidine synthase, we are analyzing trace shunt products by MS with promising preliminary results.

2) Cofactor catabolism: We have recently determined the structures of riboflavin lyase and folate monooxygenase. Cloning of the catabolic operons for biotin, lumichrome, and thiamin is in progress.

3) PLP biosynthesis: We have demonstrated that PLP synthase requires PLP-utilizing enzymes for product release. We are currently determining, the selectivity of this channeling reaction.

4)Thiamin for PET Imaging: We are collaborating with Clif Barry at NIH on the synthesis and testing of an ^{18}F -thiamin analog for thiamin-based PET imaging.

WESTON THATCHER BORDEN, CHAIR B-0027, University of North Texas.

During the past year, part of my group's research has continued an ongoing collaboration with Dr. Xue- Bin Wang at PNNL. His group measures the negative ion photoelectron spectroscopy (NIPES) of anions; and my group carries out calculations that allow us to analyze his NIPE spectra, thus providing information about the electronic structures of the neutral molecules that are formed by electron photodetachment.

One of our most recent collaborative projects involved using NIPES to investigate the transition state for the reaction of F^\bullet with HF. Dr. Wang obtained the NIPE spectrum of the F-H-F anion, and Professor Anne McCoy of the University of Washington and I performed quantum mechanical calculations, in order to analyze the NIPES spectrum and thus provide information about the F-H-F $^\bullet$ transition structure.

In another project, my long-time collaborator, Dr. David Hrovat, and I performed electronic structure calculations on the effect on the singlet-triplet energy difference of substituting the pair of oxygens in 2,7- naphthoquinone for the pair of methylene groups in 2,7-naphthoquinodimethane. We found that this substitution of two oxygens for the two CH₂ groups is actually predicted to increase the singlet-triplet energy difference, due to a switch in the ordering of the two lowest energy singlet states between these two diradicals.

Dr. Wang has obtained the NIPE spectrum of 2,7-naphthoquinone radical anion, and Dr. Hrovat and I are performing calculations in order to analyze the NIPE spectrum and thus confirm experimentally the predicted ordering of the two lowest singlet states in 2,7-naphthoquinone. The results of this combined experimental and computational study will be submitted for publication in due course.

RICHARD M. CROOKS, CHAIR F-0032, The University of Texas at Austin.

Briefly, our accomplishments in monitoring biomarkers for heart failure to date include: (1) Covalent attachment of antibodies to AgNPs; (2) Systematic investigation of the cross reactivity of selected NT- proBNP monoclonal antibodies with closely related other natriuretic cardiac biomarkers; (3) Optimization of Linear Dynamic Range (LDR) and Limit of Detection (LOD) for μ B-AgNP model composite and improvements in electrochemical detection principle; (4) Implementation of an updated physical sensor design to improve performance; (5) Preliminary implementation of a small-scale clinical trial for sensor evaluation.

In our electrocatalysis research, we have shown that density function theory (DFT) can be used to accurately understand how Au nanoparticle (NP) catalysts cooperate with SnO_{1.7} and SnO_{2.0} supports to carry out the oxygen reduction reaction (ORR). That is, theoretical calculations and experimental results agreed that both SnO_{1.7} and SnO_{2.0} supports have strong enhancing effects on the ability of AuNPs to electrocatalyze the ORR. Specifically, in the case of AuNP interaction with a SnO_{1.7} support, the number of electrons involved in the ORR (n_{eff}) increased from 2.1 ± 0.2 to 2.9 ± 0.1 , while the onset potential decreased by 0.320 V. Similarly, direct interactions between AuNPs and a SnO_{2.0} support, led to an improvement in the n_{eff} from 2.2 ± 0.1 to 3.1 ± 0.1 and the reduction of the onset potential by 0.280 V. These experimental results are in excellent agreement with the theoretically predicted onset potential shift of 0.30 V. Therefore, this is a rare case of theory leading to nearly perfect agreement with experimental electrochemical results.

The accomplishments in our desalination project include development of an in-situ conductivity measurement to quantify separation, simplification of the separation platform, and development of a better understanding of the separation process itself.

OLAFS DAUGULIS, CHAIR E-0044, University of Houston.

1. We have developed a method for cobalt-catalyzed, carboxylate-directed functionalization of arene C-H bonds. Alkynes, styrenes, and 1,3-dienes are coupled with benzoic acids to provide cyclic products in good yields. The reactions proceed in the presence of a cobalt(II) hexafluoroacetylacetonate catalyst, amine base, Ce(IV) co-oxidant, and oxygen. Currently, this is the most general method for carboxylate-directed C-H functionalization by first-row transition metal catalysts.

2. A general method for synthesis of 1,2-bis-trifluoromethylthioarenes has been developed. Arynes generated from silyl aryl triflates or halides react with bis(trifluoromethyl)disulfide to afford 1,2-bis-trifluoromethylthioarenes. Aryl, alkyl, ester, halide, and methoxy functionalities are compatible with reaction conditions. Method is applicable for the modification of biologically active compounds.

3. In collaboration with Dr. Coates' group at Cornell, we have reported a ¹³C NMR study of poly(α-olefins) using a series of diimine-nickel catalysts. A mathematical model capable of quantifying the ¹³C NMR data into eight unique insertion pathways was developed. With this model, overall regiochemistry

of insertion and overall preference for primary versus secondary insertion pathways using nickel diimine polymerization catalysts under various conditions was determined. The model provides the tools necessary for determining how ligand structure and polymerization conditions affect catalyst behavior for α-olefin polymerizations.

4. Several new olefin polymerization systems were developed and the corresponding reaction mechanisms were investigated in collaboration with Dr. Brookhart's group. Specifically, comprehensive synthetic and mechanistic studies of the α-diimine nickel-catalyzed copolymerizations of ethylene and vinyltrialkoxysilanes, including low-temperature NMR studies of intermediates, were performed. A complete description of the chain growth process was provided.

LUIS ECHEGOYEN, CHAIR AH-0033, The University of Texas at El Paso.

Welch support was acknowledged in 13 articles, ranging in research topic from empty and endohedral fullerene functionalization to Solar Cells. One article was published in Nat. Commun., one in JACS, three in J. Mat. Chem. (A, B and C), one in Angew. Chem. Int. Ed. and one in Chem. Mat.

The uranium-based endohedral fullerene project yielded the first fully characterized dimetallic endohedral compound, U₂@Ih-C80, including its single crystal X-Ray structure. Calculations for this endohedral dimetallic compound predicted a weak bond between the two U ions, with a distance of 3.9 Å. Interestingly the crystallographically determined internuclear distance was 3.72 Å, shorter by 0.2 Å, indicating a slightly stronger bond between the U ions. More recent results, just accepted for publication in Nat. Commun., provided full characterization for a totally unexpected and never even theoretically considered compound, U₂C@Ih-C80. The unprecedented and ordered U=C=U cluster exhibits two well defined U=C double bonds with lengths of 2.03 Å, making them the first ever well characterized double bonds between U and C. The fullerene cage serves as a stabilizing nanocontainer inside which highly reactive clusters can exist. Once formed the endohedral compounds are completely stable, thermally and chemically. Besides the novel carbide cluster we have also detected U₂N, U₂O and U₂S species encapsulated in different fullerene cages. Future work will concentrate on the synthesis, purification and characterization of these novel compounds and in understanding the fundamental bonding interactions between U and these elements. We will also focus on the isolation of other U₂C@C_{2n} compounds (2n = 72 and 78, already detected) and U₂@C_{2n} (2n = 72 and 78, also detected).

We also continued to make considerable progress (four publications) with hybrid inverted perovskite solar cells, using a variety of fullerene and some non-fullerene compounds as selective electron extracting layers.

J. RUSSELL FALCK, CHAIR I-0011, The University of Texas Southwestern Medical Center.

In synthetic methodology, we reported: (1) the rt, rhodium-catalyzed insertion into unactivated C-H bonds. The reaction is highly distereoselective and provides good access to pyrrolidines. (2) An inexpensive, environmentally friendly, and stereospecific cross-coupling of α-alkoxyalkylstannanes with organic electrophiles was achieved using MnCl₂ alone or in combination with copper salts. In collaborative medicinal/biological studies, we: (1) described the upregulation of 20-HETE synthetic cytochrome P450 isoforms in cortical neurons by oxygen and glucose deprivation that directly contributes to neuronal death; (2) reviewed the development of orally epoxyeicosatrienoic acid (EET) analogs and their advancement towards clinical applications; (3) showed a new class of biguanides bind to cytochrome 3A4 and inhibit breast cancer mitochondria and EET biosynthesis, opening a potential cancer therapy; (4) disclosed CypP450 epoxides of eicosapentanoic acid and stable synthetic analogs led to significant resolution of choroidal neovascularization associated with age-related macular degeneration; (5) confirmed using Cyp4a14(-/-) mice that the blood pressure lowering effect of 20-hydroxyeicosatetraenoic acid (20-HETE) blockade is due to renal natriuresis; (6) established that increases in blood flow in the rat adrenal gland in vivo induced by angiotensin II (Ang II) are mediated by release of nitric oxide (NO) and EETs, whereas increases by adrenocorticotrophic hormone (ACTH) are mediated by EETs alone; (7) showed M2, but not M1, macrophages degrade 12(S)-hydroxyeicosatetraenoic acid [12(S)-HETE] into hydroxylated products that no longer enhance ANG II-induced vascular constriction, supporting an antihypertensive role for M2 macrophages; and (8) demonstrated two pharmacological EET-enhancing therapies effectively exert antihypertensive effects and can reduce the severity of ischemic arrhythmias in rats with Ang II-dependent hypertension.

CHARLES P. FRANCE, CHAIR AQ-0039, The University of Texas Health Science Center at San Antonio.

In response to the ongoing opioid epidemic and a call from the NIH for new approaches to treat opioid abuse and overdose, we are studying and developing methocinnamox (MCAM), a novel, pseudoirreversible, μ opioid receptor antagonist. MCAM has pharmacological properties that might be

preferable to currently available medications for treating opioid abuse (naltrexone, buprenorphine, and methadone) or overdose (naloxone). Because MCAM has no agonist properties, it avoids the diversion, abuse, and potentially lethal effects (respiratory depression), including serious drug interactions, that can occur with the opioid agonist replacement therapies buprenorphine and methadone. Because MCAM dissociates very slowly if at all from μ opioid receptors, it has a much longer duration of action than naltrexone or naloxone and, unlike the competitive reversible antagonists naltrexone and naloxone, the antagonist properties of MCAM are not overcome by taking more agonist. Our studies in monkeys show that a single injection of MCAM reverses and protects against the respiratory depressant effects of heroin for several days. A single injection of MCAM also blocks intravenous self-administration of heroin, but not cocaine, for a week or longer. Given these exciting results and the excellent safety profile of MCAM in vivo and in vitro, we filed a US patent application and submitted several NIH grants to facilitate the further characterization and development of MCAM, not only for opioid abuse but also to protect military and law enforcement personnel as well as civilians from the weaponization of opioids (e.g., ultra-potent fentanyl analogs). This year we were awarded two new NIH grants to study drug mixtures that include the anti-obesity drug lorcaserin (Belviq®), in one case with buprenorphine (Buprenex®) for treating opioid abuse and in another case with the anti-anxiety drug buspirone (Buspar®) for treating stimulant abuse.

ANDREW FUTREAL, CHAIR G-0040, The University of Texas M.D. Anderson Cancer Center.

We have continued work in the lab focused on tumor heterogeneity and how genetic variation affects clinical biology, with an emphasis on longitudinal approaches. We have completed our work on relapsed/refractory osteosarcoma that is being readied for publication. Similarly, we are nearing submission for publication of our whole tumor ecosystem heterogeneity work, incorporating (in addition to reconstruction of an entire lesion) multiple longitudinal samples over a 10-year clinical course from the patient. This work is providing unique insights into multiple mechanisms of resistance, the nature of immune control and recurrent, indolent disease. In addition to these efforts approaching fruition, we have continued to pursue multiple cancer genomics/genetics projects. Of note, the work we have done understanding mutations of the SWI/SNF complex and its therapeutic implications in lung cancer were recently published in Nature Medicine. Our continued work on the longitudinal analyses of leukemia led to the publication of a study detailing the impact of clearing mutations after induction chemotherapy on subsequent relapse in acute myeloid leukemia in the Journal of Clinical Oncology. In keeping with another emphasis in the lab – that of studying rare cancers - we recently published the first detailed molecular characterization of adult mixed phenotype acute leukemia in Nature Communications. This work will have impact on the appropriate diagnosis and treatment choices for this subset of leukemia patients. As in previous years, we have endeavored to leverage the important support of the Welch Foundation in key areas of emphasis centered on deep molecular analyses of clinically relevant questions with a focus on longitudinal studies and rare cancers. The over-arching theme of the role of tumor heterogeneity in impacting clinical heterogeneity and how this can be prosecuted for ultimate patient benefit remain the key tenants that are empowered by the Welch funding.

VADIVEL GANAPATHY, CHAIR BI-0028, Texas Tech University Health Sciences Center.

During the past funding period, we published five reviews and two original papers: (i) Cell-surface and nuclear receptors in the colon as targets for bacterial metabolites and its relevance to colon health; (ii) Short-chain fatty acid transporters: Role in colonic homeostasis; (iii) Tooth hypoplasia for differential diagnosis of childhood epilepsy associated with SLC13A5 mutations; (iv) The Na⁺/Cl⁻-coupled, broad-specific, amino acid transporter SLC6A14 (ATB0,+): Emerging roles in multiple diseases and therapeutic potential for treatment and diagnosis; (v) Transporter-guided delivery of nanoparticles to improve drug permeation across cellular barriers and drug exposure to selective cell types; (vi) Dual targeting of L-carnitine-conjugated nanoparticles to OCTN2 and ATB0,+ in cancer cells to deliver chemotherapeutic agents for colon cancer therapy; and (vii) L-Carnitine-conjugated nanoparticles to promote permeation across blood-brain barrier and to target glioma cells for drug delivery via the novel organic cation/carnitine transporter OCTN2. Progress in the current grant year includes: (a) Use of cell-surface transporters for delivery of drugs in the form of nanoparticles; (b) Analysis of colonic bacteria and transcriptome profile in wild type mice and Slc5a8-null mice on either a high-fiber diet or a low-fiber diet; (c) Hfe-null mice have increased uric acid in plasma and tissues, partly due to down regulation of the urate efflux transporter ABCG2; (d) -Methyltryptophan reduces colon cancer in a syngeneic transplant model; and (e) Gpr81, a cell-surface receptor for lactate, plays a paracrine role to promote breast cancer.

JAN-ÅKE GUSTAFSSON, CHAIR E-0004, University of Houston.

1. We have created a new ERbeta ko mouse by deleting the ER gene with crispr/cas9. The phenotype of the new knockout mouse is very similar to that of the original Oliver Smithies mouse in the prostate, mammary gland, ovary, and brain.
2. We have discovered a role for ERbeta in the development of the central nervous system. We used mouse ES cells in culture and found that in the absence of ERbeta cells differentiate into oligodendrocytes rather than neurons. Thus ERbeta plays a key role in early brain development.
3. We have been intensively investigating the role of ERbeta and its splice variants in breast and prostate cancers. We found that ERbeta 1 and ERbeta 2 are expressed in 20-30% of triple-negative breast cancers, and that treatment of patient derived TNBC xenographs respond to an ERbeta agonist by a reduction in invasiveness but had no effect on proliferation.
4. In cell lines, ERbeta splice variants, ERbeta2, ERbeta4, and ERbeta5 exert effects on proliferation which are opposite to those of ERbeta, and are markers of poor prognosis in cancers while ERbeta1, confers sensitivity to chemotherapy
5. We have discovered a very unexpected use for ERbeta-selective agonists. It is to increase the number of neurons in the myenteric plexus after neuronal loss by injury from a high fat diet or chemical destruction.
6. We have discovered a role for LXRbeta in lamination of the dentate gyrus and shown that loss of LXR leads to autistic like behavior in mice.

7. In addition, knockout of LXRbeta in astrocytes led to astrogliosis in the habenular nucleus and this offers a new explanation of the loss of dopaminergic neurons in the substantia nigra which is the phenotype of the LXRbeta ko mice.

8. Most rewarding and potentially very important is our very recent data showing that in the APP mouse (a mouse overexpressing amyloid precursor protein), treatment with an ERbeta-selective agonist led to reduction in the number of beta amyloid plaques.

WILLIAM L. HASE, CHAIR D-0005, Texas Tech University.

Progress was made in development of models, algorithms, and computer programs for chemical dynamics simulations, and in application of this software to significant research problems. The Hase research group continues to develop the VENUS computer program for performing chemical dynamics simulations. They also develop, maintain, and distribute the VENUS/NWChem software package for direct dynamics simulations. The Hase research group maintains the Chemical Dynamics Software and Simulation portal <http://cdssim.chem.ttu.edu> for: 1. Distributing VENUS and other chemical dynamics software; 2. Providing graphical user interface (GUI) tools for modifying and building simulation models; 3. Providing a repository of chemical dynamics software and simulation models used by the Hase group. This portal is a valuable tool for other research groups and scientists. Support from the Robert A. Welch Foundation is acknowledged. The specific research problems reported here are: 1. Competing E2 and SN2 dynamics; 2. Dynamics of gas-phase SN2 reactions, including microsolvation; 3. Post-TS and unimolecular dynamics; 4. Development of algorithms and software for chemical dynamics simulations (including direct dynamics); 5. Theory of unimolecular and intramolecular dynamics; 6. Intermolecular potentials and dynamics for interactions of peptide ions with organic surfaces; 7. Use of a liquid and gas phase model to study gas phase intermolecular energy transfer; 8. Thermal and collision-induced dissociation (CID) of peptide ion fragmentation; 9. N2 and O2 collisions with graphite; 10. PSO algorithm for fitting analytic potential energy functions; 11. Synthesis of biological molecules in the interstellar medium; 12. Dynamics of the 3CH2 + 3O2 reaction; 13. Anharmonic sums and densities of state; Animations of these simulations are available on the portal <http://hase-group.ttu.edu/>. They are used by national and international scientists for both teaching and research.

ALLAN J. JACOBSON, CHAIR E-0024, University of Houston.

Recently, we have synthesized V(OH)ndc·H2O (ndc = 2,6-naphthalenedicarboxylate) and determined its structure by single crystal X-ray diffraction. Anhydrous V(OH)ndc and VOn dc were obtained from V(OH)ndc·H2O in crystal to crystal transformations and their structures determined. The VOn dc phases all exist in the narrow pore form unlike the aluminum analog (MIL-69), which exists as both narrow pore (np) and large pore (lp, DUT-4) structures. A likely explanation for the closed structure of V(OH)ndc·H2O is rotation of neighboring VO6 octahedra along their axial axis, which destroys the nearly coplanar relationship of the two V-O bonds to each carboxylate group. The coplanarity is necessary for a hinge-like geometry required by breathing deformations as found in MIL-47. If the template water molecules are responsible for channel closing and the relative rotation of the octahedra, other non-water templates may favor large pore frameworks. We have shown that the use of non-aqueous solvents in the synthesis does give large pore V(OH)ndc. In other work, we have demonstrated a one-step strategy for the formation of several non-proteinogenic amino acid-metal complexes containing racemic mixtures of the chiral ligands. As an example, the hydrothermal reaction of (E,E)-muconic acid, ethylenediamine and nickel chloride hexahydrate gave Ni(rac-piperazine-2,3-diacetate)(H2O)2. Under mild hydrothermal conditions, the piperazine-2,3-diacetate anion is formed through Michael addition of the amine group of ethylenediamine to muconic acid followed by intramolecular Michael reaction with the other amine group. The structure consists of chains in which nickel atoms are alternately bridged by racemic piperazine-2,3-diacetate anions. Two coordinated water molecules complete the structure of Ni(rac-piperazine-2,3-diacetate)(H2O)2. The chains are connected by hydrogen bonds. Demetallation to generate the corresponding non-proteinogenic amino acid can be achieved by acidic hydrolysis.

THOMAS KENT, CHAIR-BE-0048, Texas A&M University Health Science Center.

I was recently appointed to the Welch Chair BE0048 on February 5th, 2018. As of May 31, 2018 there has not been any activity on this grant.

MICHAEL J. KRISCHE, CHAIR F-0038, The University of Texas at Austin.

In the 2017-2018 funding period, numerous advances were made. Exploiting the concept of transfer hydrogenative coupling pioneered in by Professor Krische (Acc. Chem. Res. 2017, 50, 2371), a ruthenium(0)-catalyzed cycloaddition of benzocyclobutenones that functionalizes two adjacent saturated diol carbon-hydrogen bonds was developed (Science 2017, 357, 779). An enantioselective variant of this process was subsequently developed and is pending review. These regio- and diastereoselective processes contributing to a growing body of metal catalyzed cycloadditions mediated by hydrogen transfer developed in the Krische laboratory (Review: Angew. Chem. Int. Ed. 2018, 57, 3012). Using Professor Krische's catalytic C-C couplings, methods for the synthesis of phthalide natural products were developed (Angew. Chem. Int. Ed. 2018, 57, 1390) and progress toward the total synthesis of the antimicrobial marine macrolide leiodermatolide was made (Org. Lett. 2017, 19, 6634). Two major review articles related to Professor Krische's research were published (Chem. Rev. 2017, 117, 12564; Chem. Rev. 2018, 118, In Press). Beyond contributions to existing lines of investigation, Professor Krische's laboratory has entered broad, new areas of research. For example, the synthesis of helical rod-like phenylene cages (J. Am. Chem. Soc. 2018, 140, 2455) and the development of catalytic C-N bond forming processes (J. Am. Chem. Soc. 2018, 140, 1275). During the 2017-2018 funding period, Professor Krische was elected to the American Association for the Advancement of Science (AAAS).

JAMES C. LEE, CHAIR H-0013, The University of Texas Medical Branch.

As a consequence of integrating computation, high resolution structural analysis and quantitative dissection of the linked functional equilibria a quantitative structure-function correlation for an allosteric transcription factor, namely, *E. coli* cAMP receptor protein (CRP), is emerging. The computation algorithm COREX/BEST provides residue stability constants of CRP based on crystallographic structures determined under different experimental conditions with known changes in allosteric behaviors. Furthermore, the connectivity among residues is also defined hence it is possible to establish the change in structural landscape in terms of G . Simultaneously, the energetics of ligand binding which serves as allosteric activation for DNA binding are also defined by calorimetry or other spectroscopic approaches.

Studies include pH, salt, temperature dependence or mutations of single residues. The allosteric behavior ranges from negative to positive cooperativity in cAMP binding with the switch over point at defined pH, temperature and salt concentration. The residue stability constants are experimental conditions, particularly those associated with the A subunit. The origin of the dominant change is the DNA binding domain specifically of the B subunit. Although CRP is a homo-dimer, these dimers are asymmetric exhibiting different patterns of B-factor and stability constants of residues. The A subunit stability and B- factor patterns are not significantly perturbed by pH or the other experimental conditions but that of the B subunit do, particularly the DNA binding domain. Thermal stability of the cloned DNA binding domain is pH, salt concentration and temperature dependent following the same stability pattern as that derived from COREX based on the crystal structures available. Hence, there is a strong quantitative correlation between structural and functional landscapes. There are correlations between stability constants of residues and functional energetics.

DAVID D. MOORE, CHAIR Q-0022, Baylor College of Medicine.

Our focus is on the roles of nuclear receptors in cell stress pathways, and much of the progress over the last year was based on liver stress. In the manuscript by Kim et al (PMID: 28378930) we discovered an unexpected metabolic benefit in mice undergoing severe and chronic elevations of toxic bile acids due to loss of function of the bile acid homeostatic axis mediated by the nuclear receptors SHP and FXR. At older ages these double knockout (DKO) mice showed improved glucose and fatty acid homeostasis, reversing the aging phenotype of body weight gain, increased adiposity, and insulin intolerance, suggesting a central role of this axis in whole-body energy homeostasis.

We also showed that the DKO mice are similar to human patients with genetic syndrome PFIC-5 (Progressive Familial Intrahepatic Cholestasis – 5) in that they show to activation of the pathway of drug metabolism, which is mediated by the nuclear receptors CAR and PXR (PMID:29718219). In contrast, such activation is absent in both human patients with PFIC-2 and the corresponding mouse model of the disease. These results provide a deeper understanding of the heterogeneity of intrahepatic cholestasis.

BRUCE J. NICHOLSON, CHAIR AQ-0012, The University of Texas Health Science Center at San Antonio.

We had run a prior search to fill this position and identified an excellent candidate, but ultimately he decided to accept a very large retention package from his home department. Thus, we re-posted the position and advertised in Science (October costs). We obtained 15 unsolicited applications, as well as one from Dr. Patrick Sung who we encouraged to apply after we learned that he was interested in moving from his current position at Yale. We interviewed two candidates (including the solicited application from Yale), and hosted them for visits/seminars in January, for which we used the Welch funds combined with Cancer Center resources. Dr. Patrick Sung, was our unanimous choice, and was offered the position, and a CPRIT Scholar recruitment Award was submitted on his behalf and funded at \$6M. As part of his recruitment, we also interviewed one of the senior researchers in his lab (Dr. Weixing Zhao) for a faculty position (also covered from Welch funds). We were impressed by the quality of Dr Zhao's work, and his independence, and have also tendered him an offer, which he has recently indicated he will accept. Thus, the accrued balance has been used effectively and judiciously to recruit two outstanding faculty, particularly Dr Sung who served for 6 years as Chair of Biochemistry at Yale and has established a stellar career in DNA repair. The unexpended balance in the Welch Chair account will be used to develop the research program of Dr. Sung once he arrives in January, 2019. His protege, Dr. Zhao, is expected to arrive in December 2018.

ERIC N. OLSON, CHAIR I-0025, The University of Texas Southwestern Medical Center.

During the past year, we discovered that the Kelch proteins Kih131 and Kih141 are required for skeletal muscle growth and function by controlling the degradation of various muscle contractile proteins. Mice lacking these Kelch proteins exhibited stunted postnatal skeletal muscle growth, lethal myopathy, and sarcomere disarray. Our findings provide new insights into the molecular basis of human congenital myopathies and suggest biochemical strategies for ameliorating muscle disease.

We discovered a micropeptide, named MOXI (Micropeptide regulator of β -oxidation), which localizes to the inner mitochondrial membrane where it regulates mitochondrial metabolism and energy homeostasis and thereby enhances muscle function and exercise tolerance. In general, our studies underscore the regulatory potential of additional micropeptides that have yet to be identified. We are continuing to explore several such micropeptides.

We also continued to optimize methods for correction of mutations in the dystrophin gene responsible for Duchenne muscular dystrophy (DMD). We optimized the viral delivery of CRISPR/Cas9 gene editing components to muscle and heart using mouse models of DMD. In addition, we devised a strategy to correct a wide spectrum of human DMD mutations using induced pluripotent stem cells as a model system. We are currently advancing these studies into large animals as a prelude to eventual clinical translation.

As a means of repairing the heart following myocardial infarction (MI), we performed an unbiased screen of transcription factors for those that can promote the conversion of adult fibroblasts into cardiomyocytes. We discovered that the zinc finger transcription factor 281 (ZNF281) potently stimulates

cardiac reprogramming by genome-wide association with the GATA4 transcription factor on cardiac enhancers. We are currently further optimizing this approach for cardiac regeneration.

RODERIC PETTIGREW, CHAIR BE-0023, Texas A&M University Health Science Center.

I was recently appointed to the Welch Chair BE#0023 on November 1, 2017. As of May 31, 2018, there has not been any activity on this grant. Hiring a research post Doc is planned to help initiate this work in collaboration with the Cooke Laboratory at Houston Methodist Research Institute.

B. MONTGOMERY PETTITT, CHAIR H-0037, The University of Texas Medical Branch.

Modern theories of the liquid state are well challenged in application to macromolecules such as proteins and nucleic acids. We employ analytic theory as well as computer simulation to consider how the interatomic interactions give rise to the thermodynamic behaviors of such systems. In an ongoing study we have considered the mechanism of how the shapes and conformational distributions of polypeptides are affected by the balance between aqueous solvation and intramolecular interactions. We found that dipolar interactions among carbonyls rather than hydrogen bonds dominated systems which were disordered. We found this same unexpected mechanism to dominate the solubility limit of peptides. We found the results to be independent of force field used to describe the potential energy surface. The liquid-liquid phase separation that characterizes the solubility limit for small peptides we discovered to be also driven by the same non-hydrogen bonding interactions. Thus, both in a single peptide as well as in separated liquid phases these disordered systems use a different aspect of the dipolar interaction surface than the traditional hydrogen bonds to achieve a thermodynamic equilibrium state. We have characterized the solvation thermodynamics including the free energy per particle or chemical potential and entropy for these peptide systems. The difference between the flexible system and a single rigid conformer should represent the free energy and entropy difference due to flexibility. We were able to check this explicitly by calculating the conformational entropy explicitly for a range of systems. We found the entropy scales essentially linearly with the number of amino acid residues for these disordered systems. We have applied these fundamental insights to other protein containing systems such as viruses where order-disorder transitions play an important role.

LASZLO PROKAI, CHAIR BK-0031, University of North Texas Health Science Center.

In this reporting cycle, the most significant progress I made in my research objective was the identification of estrogen-regulated proteins and protein networks in the retina that is an integral part of the mammalian CNS. Using an animal model (ovariectomized female Brown Norway rats treated for about three weeks with daily eyedrops of 17 β -estradiol, E2) and a mass spectrometry-based proteomics approach relying on label-free quantification, I have identified 63 E2-regulated proteins upon comparing retinal protein levels in treated versus vehicle-control groups. Specifically, I found that the female hormone up-regulated 46 proteins and down-regulated 17 proteins in the rat retina. Most importantly, I have been able to map them by Ingenuity Pathway Analysis (Qiagen) to protein networks also identifying functions and pathways represented by them, which has been unprecedented thus far in the scientific literature regarding estrogen-regulated retinal proteins. Functions associated with the most prominent network I built (by merging two overlapping networks) included cell-to-cell signaling and interaction, cellular assembly and organization, as well as DNA replication, recombination and repair, gene expression and cell cycle. In addition, I built another significant network with associations to small-molecule biochemistry, specifically involving lipid, carbohydrate and nucleic acid metabolism (with the tricarboxylic acid cycle and oxidative phosphorylation as the associated principal biochemical processes), and also to cell morphology. Altogether, my findings will be a treasure trove of data for the scientific community of eye researchers. In particular, this work may facilitate the discovery of potentially druggable targets regarding treatment of ophthalmic maladies after the planned publication of the completed study, along with the raw data files also deposited to the ProteomeXchange online resource, as soon as the comprehensive evaluation of the results is finished.

JAMES SACCHETTINI, CHAIR A-0015, Texas A&M University.

The major emphasis of the laboratory is on antimicrobial drug-resistance and drug discovery. These longstanding efforts on structure guided drug discovery have led to several lead molecules that targets *M.tuberculosis*. We have teams of medicinal chemists, structural biologists, and our high throughput screening facility to the goal of developing leads against novel drug targets. We are also working on the *Mtb* ribosome and RnaP, both validated antibiotic targets. In addition, we have completed a high resolution Cryo-EM structure of the *Mtb* ribosome to complement developing drugs that efficiently inhibit *Mtb* translation.

Another area of particular importance is the development of a clinical candidate that targets the acetyl CoA carboxylase of *Cryptosporidium*, the parasite that causes cryptosporidiosis. Cryptosporidiosis is responsible for significant infant mortality in developing countries because there are no effective drugs against it. We have developed leads that are extremely potent, several with anti-parasitic activity in the picomolar range. They show no detectable toxicity and great efficacy in *in vivo* mouse and calf models of infection, and our current lead is being evaluated for clinical trials.

We have developed novel rifamycins that are extremely efficient at sensitizing drug resistant cancers to standard chemotherapeutics. RTI-79 has a broad spectrum of action that includes ovarian cancer and double and triple hit non-Hodgkin's lymphoma. They increase the sensitivity of resistant ovarian cancer (NCI/ADR-RES) to doxorubicin by over 800-fold. In fact, they synergize with many different chemotherapeutics in various cancers, restoring drug sensitivity. We have recently discovered that RTI-79, also sensitizes radiation resistant prostate cancer cells to radiation. RTI-79 is non-toxic and has favorable *in vivo* safety and pharmacokinetic profiles. RTI-79 in combination therapies is effective in multiple drug-resistant cancers in mouse models.

KIRK SCHANZE, CHAIR AX-0045, The University of Texas at San Antonio.

In November 2017 – January 2018 an ultrafast fluorescence spectroscopy system was installed that was funded by the Welch Chair funds. This system comprises a Coherent Chameleon Ti-sapphire oscillator source combined with a PicoQuant FT300 time-correlated single photon counting fluorescence spectrometer. This system has the capability of measuring fluorescence spectral dynamics over 350 – 800 nm range with time resolution from 20 ps – 100 us. This system will be utilized for a number of projects in the Molecular and Materials Photoscience Laboratory.

Dr. Amanda Sulicz joined the group in September 2017 as a postdoctoral associate supported by the Welch Chair after receiving her Ph.D. from Case Western Reserve University. Amanda's research is focused on the study of fundamental excited state properties of organometallic chromophores that contain electron donor-acceptor conjugated pi-electron systems. Her work comprises synthetic organometallic chemistry, and photophysics. To date Amanda has accomplished the synthesis and characterization of three unique compounds and she has carried out detailed photophysical analysis of the same. Her preliminary results will be presented at the Gordon Research Conference on Electron Donor-Acceptor Interactions in August 2018.

The group also completed and submitted for publication five research papers that acknowledge Welch Foundation for partial support.

GUSTAVO E. SCUSERIA, CHAIR C-0036, Rice University.

During the past year, we have continued developing novel quantum chemistry methods. Our focus remains on methodology for both molecules and systems with periodic boundary conditions (surfaces and bulk materials), and it involves both density functional and wave function methods. Our main efforts have focused on symmetry breaking and restoration techniques, particularly their combinations with novel forms of coupled cluster theory, the leading paradigm in quantum chemistry. For solid state systems, we have continued developing a quantum embedding theory based on the one-particle density matrix. Details and results associated with the research projects are provided in the list of publications accompanying this report.

JONATHAN SESSLER, CHAIR F-0018, The University of Texas at Austin.

During this period as the Doherty-Welch Chair at The University of Texas at Austin, we continued preparing and developing novel systems capable of self-assembly via anion and ion pair recognition, and molecular sensing. An effort was devoted to the preparation of novel expanded porphyrins and their metal complexes. A new expanded porphyrin, hexadecaphyrin was obtained via condensation of a hexapyrrolic derivative, which exhibits a weakly antiaromatic character. The bis-cobalt(II) complex displayed two different conformers with distinct spectral optical features that are temperature dependent. This expanded porphyrin bis-cobalt(II) complex was proposed as a potential tunable thermal sensor. Another pi-expanded macrocycle synthesized during the funding period was a 26 pi-electron-expanded porphycene; this system proved capable of coordinating two rhodium cations within a Huckel-type aromatic framework. This proved true for both the free base and bimetallic complex.

We also focused on exploring the self-assembly properties of a carboxylic acid-functionalized "Texas- sized" molecular box. In this case, functionalization of the tetracationic imidazolium-based box led to the formation of dimers paired in a clip-like fashion. However, altering the conditions led to self-assembly into an oligomeric arrangement with the key determinants being pH and concentration. Incorporating this macrocycle into hydrogels with specific fluorophores resulted in a responsive hydrogel whose features could be varied through exposure to various chemical stimuli. This latter work was highlighted in Nature: www.nature.com/articles/d41586-018-01139-6. Hydrogels containing the "Texas-sized" box were also used for the removal of anions from aqueous media. The remarkable versatility of this new method was highlighted in the in the online version of C&E News: <https://cen.acs.org/articles/96/web/2018/03/Hardy-hydrogel-cleans-water.html>.

ERIC E. SIMANEK, CHAIR P-0008, Texas Christian University.

Almost two decades of chemistry focused on the exploration of dendrimers based on triazines have come to an end. Two manuscripts were published. The first described the "facile synthesis of stable, water soluble, dendron-coated gold nanoparticles" wherein dendrons with a diazonium salt at the focal point were mixed with gold trichloride and treated to reductive conditions to yield the product. Computational models were used to rationalize solubility and anchor our intuition of structure of these products. This report appears in the journal "Nanoscale." A second manuscript reported that "intrinsic fluorescence of triazine dendrimers provides a new approach to study dendrimer structure and conformational dynamics." The results confirm a structural transition in triazine architectures occurring between generation 3 and generation 5 materials that is consistent with other scaffolds described in the literature. The methods corroborate and anchor previously under-substantiated reports of a "sweet spot" of activity in many biological applications. This report appears in the "Journal of Physical Chemistry."

As a departure from multistep organic synthesis aimed at large molecule targets, the focus of the laboratory has shifted to self-assembly of small molecules through the formation of reversible, labile linkages. Leveraging our experience with triazine chemistry, hydrazine-derivatized molecules were condensed with carbonyl donors including aldehydes, ketones, and 1,3-diketones. The initial report of mono-carbonyl constructs appeared in the previous period. During this period, 1,3-dicarbonyls were investigated. The resulting pyrazole provides a largely irreversible linking strategy. In the process of exploring this chemistry, however, we have discovered routes and design criteria to stable hemiaminals. The chemistry of this functional group is being explored currently.

JOHN L. SPUDICH, CHAIR AU-0009, The University of Texas Health Science Center at Houston.

This year we focused on the recently discovered Anion Channel Rhodopsins (ACRs). ACRs carry out a function previously unknown to occur in nature, namely light-gated channel conduction of anions (physiologically chloride). They have become widely used for photocontrol of cell membrane

electrical potential (“optogenetics”) as inhibitory tools because light-induced passive flux of chloride hyperpolarizes neuronal membranes inhibiting neuron action potentials. We aim to elucidate the mechanism of ACRs both to further photochemistry and to enable ACR molecular engineering to expand their use as optogenetic tools. PART 1: Following our publication of the first two ACRs in cryptophyte algae in Science in 2015, we have now identified and characterized 32 ACR homologs. This year we emphasized structure/function analysis. We identified residues that control the rate of channel opening and closing, enabling engineering of effective neural silencing tool for processes in which high temporal control is required, e.g. for selective single-spike inhibition. We engineered an ACR with a fast closing time (2 ms halftime) to inhibit a selected single spike in a neuron firing over 100 Hz, and also ACRs with greatly extended open channel state lifetimes (up to 20 s halftime). PART 2: We have made a breakthrough by X-ray crystallographic determination of the first atomic structure of an ACR (manuscript in preparation for Science). We identified a highly expressed stable ACR, crystallized the purified protein in a photoactive form, and obtained diffraction data enabling refinement of a complete 2.9 Å-resolution structure. We are currently testing hypotheses from our analysis of the structure by mutagenesis and obtaining further crystals to elucidate the mechanism of light-gated chloride conductance by ACRs. PART 3: We completed an analysis of the cryptophyte cation channelrhodopsins that revealed a novel mechanism for control of cation conductance, and published the results in PNAS.

JOHN A. TAINER, CHAIR G-0010, The University of Texas M.D. Anderson Cancer Center.

1. Cellular stress, DNA damage responses and Cancer. We found that oxidized base repair is pre- targeted to open chromatin for genome stability (Nature under review). We aided in measuring kinetics and the energetic contributions of different components of multi-protein molecular machinery acting in DNA break repair. We published methods for employing structural avatars for inhibitor design as exemplified for MRE11. We published methods for structure determination and analysis of [Fe- S] Proteins that act in DNA repair. Specifically, we analyzed data defining the active site co-factors and functional oxidation states of type II molybdo-bis (molybdopterin guaninedinucleotide) (Mo-bisMGD) enzymes. We built a unified model for the nuclease ABC-ATPase MRE11-RAD50-NBS1 complex in orchestration of damage signaling to stress in DNA replication and repair. We combined X-ray scattering and crystallography to solve the novel dimer structure of pro-metastatic collagen lysyl hydroxylase dimer assemblies and showed that the dimer is stabilized by Fe²⁺-binding. In addition, I edited a volume on DNA damage responses and cancer and published an overview. I also organized an international Fusion conference held in Cancun on DNA Repair and Cancer.

2. Methods development for structural analyses. We are actively developing robust technologies for analyzing functionally-important structures and coupling these results to quantitative cell biology. We developed and published mathematical methods for obtaining high-resolution distance information from X- ray scattering data. In collaboration with other SAXS experts, we developed publication guidelines for the acquisition, presentation, validation, and modeling of bio-molecular X-ray scattering data. We tested X-ray scattering and cross-linking mass spectrometry (CLMS) for improving the accuracy of data assisted protein structure prediction in CASP 12.

DEVARAJAN THIRUMALAI, CHAIR F-0019, The University of Texas at Austin.

Progress Report (2017-2018):

(a) Collective migration dominates cell movement in living systems as well as in cancers. We performed simulations of tumor invasion using a minimal three-dimensional model. We discovered that cells at the periphery move with higher velocity perpendicular to the tumor boundary, while motion of interior cells is slower and isotropic. Our findings also hold in describing collective motion in growing cells and in active systems where creation and annihilation of particles play a role.

(b) Cell adhesion complexes (CACs), activated by ligand binding, play key roles in many cellular functions ranging from cell cycle regulation to mediation of cell extracellular matrix adhesion. Often, CACs are subject to mechanical force. We performed simulations to show that CACs switch from one brittle state to another as force increases much like synthetic materials. This finding has profound implications outside-in signaling in membranes.

(c) It has been realized that many proteins in humans are not structured but are disordered. However, there is no quantitative theory of their structures. We filled the gap in this key area by developing a practical way of characterizing the shapes of such proteins. The theory is general so many problems of interest in biology such as the mechanism of formation of stress granules can be understood from the perspective that we have developed. Studies along these lines are in progress.

STEVEN WEINBERG, CHAIR F-0014, The University of Texas at Austin.

During the period from 6/1/17 to the present, Steven Weinberg continued his work with Raphael Flauger of the University of California at San Diego on the effects of intervening matter on gravitational radiation from distant sources, such as gravitational waves from coalescing black holes discovered by the LIGO observatory and from quantum fluctuations in the early universe. The effects are unobservably small for known astrophysical sources but may be significant for sources in the early universe. This work has been described in a paper arXiv:1801.00386 and published in Phys. Rev. D 97, 123506 (2018).

Also, during the past year, much of Steven Weinberg’s time was taken up with commemoration of the 50th anniversary of the Standard Model of elementary particles, to which Weinberg contributed in various ways, and which is widely regarded to have started with a paper “A Model of Leptons” that he wrote in 1967. His interview with Frank Close, “Birth of a Symmetry” was published by CERN Courier in November 2017. He gave a lecture “Reminiscences of the Standard Model,” livestreamed to the International Centre for Theoretical Physics in Trieste, Italy, on October 17, 2017, and another lecture “The Rise of the Standard Models,” inaugurating the Distinguished Colloquium Series of the Brazilian Physical Society, livestreamed to Brazil on October 20, 2017. On June 4, 2018, he gave the closing talk “The Conceptual Basis of the Standard Model” at the international symposium “The Standard Model at 50” at Case-

Western Reserve University. In addition, Weinberg saw a collection of his essays "Third Thoughts" through to publication by Harvard University Press, August 2018, and has been working on a treatise "Lectures on Astrophysics" that is under contract to Cambridge University Press.

THEODORE G. WENSEL, CHAIR Q-0035, Baylor College of Medicine.

We have determined that the transduction channel of retinal ON-bipolar neurons, TRPM1 consists of two pools distinguished by reactivity in situ with different monoclonal antibodies, implying different environments and functions for the two pools. We have also found that the great majority of TRPM1 protein in the cells is not localized to the postsynaptic dendritic tips, but rather is localized within the cell body in the endoplasmic reticulum. We have also determined the structures and channel activities of two engineered variants of the channel, TRPV2, implicated in cardiovascular health and a proposed as a drug target in cancers, multiple sclerosis, and other diseases. The structures have resolutions in the range 3.6 Å – 4 Å, and revealed one in an open state, and the other in a closed state, consistent with functional measurements. The open form contained an extracellular loop known as the "pore turret," which is deleted in the closed form, pointing to a previously unknown function for this structural feature. We have also characterized the role for the Class III phosphatidylinositol-3-kinase, Vps34, in retinal pigmented epithelial cells and ON-bipolar cells. In both cases its absence causes defects in autophagy and endosome processing, and leads to cell death. However, in the retinal pigmented epithelial cells it also causes defects in processing of phagosomes, and loss of Vps34 prevents fusion of phagosomes with lysosomes.

PETER G. WOLYNES, CHAIR C-0016, Rice University.

The Bullard-Welch Chair supported trips of group members working on Welch funded projects as well as participation in meetings by Peter Wolynes. We also purchased peptide arrays to test our prediction of the structure of protein complexes involved in the formation of memory. As our publications show, progress has been made on all fronts in the last year.

JOHN L. WOOD, CHAIR AA-0006, Baylor University.

Completed the Synthesis of Aspergillin A. Aspergilline A is an oxindole containing fungal metabolite that was isolated in 2014 and has been shown to possess cytotoxic activity against a range of cancer cell lines.

Completed the Synthesis of Cyclopiamide A and Speradine E. Both cyclopiamide A and Speradine E bear structural similarities to aspergilline A and also possess modest cytotoxic activity. They were prepared by a synthetic strategies that diverges from a key intermediate prepared in our efforts toward aspergilline A.

Completed the synthesis of Several Analogs of Hippolachnin A. Hippolachnin A is a complex naturally occurring small molecule that was reported to have very interesting antifungal properties. These efforts resulted in the production of the natural product as well as several structural analogs. Eventual biological evaluation of these synthetic materials established hippolachnin A does not possess significant antifungal activity.

Completion of the Core Ring System Found in Longeracemine. Longeracemine is an interesting congener of the daphniphyllum alkaloids that was recently isolate from *Daphniphyllum longeracemosum* K. These efforts established the viability of the an [4+2] 3H-pyrrole cycloaddition approach that was inspired by the proposed biogenesis.

Preparation of Novel Staurosporine Analogs: In a project initiated in the preceding funding period we began exploring the applicability of recent advances in aryl C-H activation chemistry in preparing novel aryl substituted analogs of staurosporine.

Development of Ring Expansion Approach to N-Hydroxy-Containing Diketopiperazines: Several biologically active natural products have been isolated that possess core structures containing an N- hydroxy diketopiperazine. However viable methods for the production of this type of core structure have yet to be developed. These efforts are working to eliminate this deficiency in our current repertoire of methods.

KAREN L. WOOLEY, CHAIR A-0001, Texas A&M University.

A productive research and education program in chemistry is supported by the Welch Foundation grant, involving the design, preparation and study of unique polymer materials. The W. T. Doherty-Welch Chair in Chemistry at Texas A&M University (A-0001) supports infrastructure that is directed toward an innovative mission to educate and train a diverse community of scholars (5 undergraduates, 16 Ph.D. students, 4 postdoctoral associates, 7 senior scientists, and 1 technician), each conducting chemical research to advance the fundamental knowledge and societal application of functional polymer materials. The primary motivation is to extend the synthetic control of organic chemistry toward increasingly- complex and functional macromolecules, often by employing hierarchical approaches and relying on combinations of organic chemistry, physical chemistry, biology and engineering. The development of novel synthetic strategies, fundamental study of physicochemical and mechanical properties, and investigation of the functional performance of polymers in the diagnosis and treatment of disease, as non- toxic anti-biofouling or anti-icing coatings, as materials for microelectronics device applications, and as environmental remediation systems are targets of the research activities. With support from this Welch Foundation Chair, increasing attention has been placed on the design of these functional polymer materials with consideration of the full life cycle. Synthetic approaches to connect sugars and other natural products via labile linkages have been developed, to allow for the materials to undergo breakdown to release biologically-beneficial and environmentally-resorbable natural product small molecules. The Welch Foundation chair has been critical to each of these advances, gratefully supporting research efforts that have led to 9 peer-reviewed published articles, and 10 manuscripts submitted for publication, currently undergoing peer review or revision.

HONGCAI JOE ZHOU, CHAIR A-0030, Texas A&M University.

To expand the toolbox for Metal-Organic Material design new tools were developed aimed at controlling diffusion limitations in these materials:

1.) Linker Labelization through Thermolysis

Microporous MOFs comprise a large cross section of known MOF materials, however, the stability their high levels of connectivity and small pore-size provide are often over shadowed by kinetic limitations of diffusion through the material. To countermand this fact a new technique called Linker Labelization was devised to induce post-synthetic defects within a well ordered material. This allows for the selective inclusion of some similarly designed linker along with the original linker in a single-pot synthesis. This linker may, after material synthesis, be decomposed under controlled conditions to modify pore-size distribution.

2.) Cage Hosted Nanoparticles for Improved Catalysis

Another route to limit the diffusion issue within porous materials is to generate soluble molecular species which host a cavity designed for specific chemical reactivity. The dispersion of this species in solution decreases the diffusion issues present in multi-dimensional heterogeneous systems. A series of porous organic cages was synthesized to host ruthenium nanoparticles for dehydrogenation catalysis. The cage provides a shell which has windows for access to the active Ru core while also preventing aggregation of the nanoparticles in solution.

Further funding was used to support initial studies of the biological interactions of designed materials, general supplies, and travel related to these projects.

MISCELLANEOUS GRANTS

K-A-0002, GRADUATE RESEARCH ENDOWMENT GRANT PROGRAM, Texas A&M University.

Fifty-one fellowships were offered to superior students that applied to the chemistry graduate program. Of those offered, 26 accepted and joined the program. 25 of these students have met all departmental expectations with respect to academic progress and performance. The remaining one student had joined our program but subsequently deferred for medical reasons. The students are working on publishing their research, however, these fellowships are offered to first-year students who are not typically expected to already have publications completed at this stage.

K-C-0003, ATTWELL-WELCH GRADUATE FELLOWS PROGRAM, Rice University.

Alexander Al-Zubeidi (Link Lab) investigates the optical properties that arise from novel composite nanomaterials. Sarah Hahn (Hartkerink Lab) studies supramolecular chemistry to direct the self-assembly of novel nanostructured materials. Rachael Kress (Jones Lab) works on the design of adaptive materials with unique optical and mechanical properties. Jordan Metz (Halas Lab) researches dark field spectroscopy of aluminum nanoparticles. Alexis van Venrooy (Tour Lab) studies single wall carbon nanotubes. Phillip Baker and Aubrey Howard (Uribe Lab) focus on the mechanisms of neural crest stem cell proliferation, migration and differentiation during embryogenesis. Shikai Jin (Wolynes Lab) studies statistical characterization of systems involving a large diversity of long lived states. Xiangyu Kong and Miguel Ortiz Salazar (Warmflash Lab) use mathematical modeling to answer fundamental questions in developmental, stem cell and cancer biology. Abigail Kosgei (Phillips Lab) uses computational methods to relate the structure and dynamics of proteins to their biological functions. Xiaotong Lu (Tao Lab) focuses on two RNA virus systems: birnaviruses and influenza viruses. Yu Ouyang (Gao Lab) studies the interface of chemical biology and biomolecular engineering, focusing on small- and macro-molecule discovery. Andrea Padron and Bingyan Wu (Silberg Lab) focus on biochemical and biomolecular designs to elucidate and manipulate protein functions. Jingtong Pei (Xiao Lab) develops chemical biological tools to understand complex systems and develop novel therapeutic strategies. Xinhao Song (Shamoo Lab) explores the biophysical origins of molecular evolution to predict resistance and identify new strategies for antimicrobial therapies. Melissa Traver (Bartel Lab) uses genetic, cell biological and biochemical approaches to elucidate fundamentals aspects of plant biology. Maria Villegas Kcam (Chappell Lab) studies how RNA can be designed to create synthetic regulators of gene expression.

K-F-0001, GRADUATE RESEARCH ENDOWMENT GRANT PROGRAM, The University of Texas at Austin.

Graduate student recruiting expenses included hotel accommodations and airfare for prospective graduate student visits and other miscellaneous expenses. The assistance of the Welch Foundation was instrumental in our success at maintaining a first class program. We have continued our recruiting success with an incoming class of 43 students. This success was due in part to the Welch Foundation fellowships we can offer.

L-AU-0002, THE WELCH FOUNDATION ENDOWMENT IN CHEMISTRY AND RELATED SCIENCES, The University of Texas Health Science Center at Houston.

Carmon- Our objective is to identify and characterize unique therapeutic leads for the treatment of colorectal cancer (CRC). This year radiolabeled monoclonal antibodies (mAbs) targeting cancer stem cell receptor LGR5 were evaluated in mice as cancer diagnostics and for predicting efficacy of LGR5 antibody-drug conjugates (ADCs) using PET imaging and published these results. Furthermore, we produced and purified unique mAbs targeting GPR56, which is upregulated in CRC, and have begun assessing their potential for future ADC development.

Wang- Our objective is to define and demonstrate the role of cancer exosome-mediated cell-cell communication as the lung cancer stem cell (LCSC) niche signaling critical for lung cancer growth and metastasis. By using next-generation RNA sequencing approach, we have identified 56 miRNAs differentially expressed in lung cancer-derived exosomes, and recently demonstrated the capacity of lung cancer exosomes using miR-145-miR-371b-5p+miRNAs to support the LCSC self-renewal and tumor growth.

Narkar- Our research objective is to investigate the mechanisms by which angiogenesis or tissue vascularization is regulated, especially as it pertains to metabolic and cardiovascular diseases. This year we are reporting 3 signaling papers arising from Welch support. First publication reports the role of PGC1B in muscle wasting. Second collaborative publication is on the role of GPR110 in breast cancer. And the third publication is an invited preview on PGC1A signaling in exercise.

Gurha – Our objective is to identify the gene regulatory mechanism responsible for the cardiac phenotypes in laminopathies. This year we identified activation of novel epigenetic regulator KDM5 in laminopathies using Loss of function and Gain of function mouse models. We also identified several long non-coding RNAs that are dysregulated in laminopathies. We have one publication in preparation entitled “Lamin regulates epigenetic and non-coding RNAs in Heart”.

L-C-0003, NORMAN HACKERMAN INVESTIGATORSHIP, Rice University.

Han Xiao: Coumarin is a fluorophore with a small size, good photophysical properties and photo/chemical stability. Coumarin derivatives are widely used as imaging handles for a variety of biological assays. To generate a fluorogenic coumarin-based fluorophore, we prepared a thio-caged coumarin, in which the ester carbonyl group was replaced by a thiocarbonyl group. A simple substitution of the coumarin oxygen atom with a sulfur atom leads to an efficient photoinduced electron transfer (PET), thus quenching the fluorescence. To restore the fluorescence, the thiocarbonyl group can be desulfurized to its oxo analogues under the oxidative conditions. The synthesized thiocoumarin exhibited almost no fluorescence, but would be readily converted back to its coumarin analogue upon irradiation in air. To determine the turn-on efficiency, the photoactivation of thiocoumarin was carried out using a 254 nm-hand-held UV lamp. A complete conversion to the coumarin was achieved within 2 mins.

Matt Jones: The first year of the Jones Lab primarily involved establishing the key experimental capabilities to accomplish the research objective. This required nanoparticle characterization equipment, such as a UV-vis-NIR spectrophotometer, and nanoparticle synthesis equipment, such as Schlenk lines and a glovebox. With these tools, a variety of nanoparticle building blocks have been synthesized and functionalized with surface ligands to probe questions regarding systems-level assembly phenomena. For example, silver triangular prism particles have been synthesized that are ~ 5 nm in thickness and ~1 um in edge length. At these high aspect ratios, the particles become extremely flexible and can be deformed around other nanostructures on surfaces or in solution. This observation suggests that well-controlled mechanical deformation can be used as a new paradigm for controlling the plasmonic properties of metal nanoparticles and the optical emission of semiconductor nanoparticles.

L-C-0004, J. EVANS ATTWELL-WELCH POSTDOCTORAL FELLOWSHIP ENDOWMENT IN CHEMISTRY, Rice University.

Oara Neumann: Last year's research focused on engineering a compact, near-infrared plasmonic nanostructure integrated with dual image-enhancing agents: T1-weighted magnetic resonance imaging (MRI) and fluorescence optical imaging (FOI) agents, to visualize tumors and monitor treatment efficacy during and after therapy. We use a multilayer core-shell nanostructure that consists of an Au core, silica spacing layer, and an outer Au shell that can be functionalized with targeting agents, drug payload, and polyethylene glycol (PEG). Metal ions such as Gd³⁺, Fe³⁺, and Mn²⁺, together with appropriate fluorescent dyes, were embedded in the silica layer, enhancing both optical-and MR-imaging characteristics. The internalization of Gd(III) within the Au-coated NM (Gd-NM) reduces the potential for exposure of Gd(III) to the patient. This method of T1 enhancement is even more effective for Fe(III), a potentially safer contrast agent.

Qingfeng Zhang: We used single-particle circular differential scattering (CDS) spectroscopy to quantitatively investigate the origin of plasmonic circular dichroism (PCD) from nanoparticle-protein complexes, in which the Au nanorod-bovine serum albumin (BSA) complex was chosen as a model system. We demonstrated that single Au nanorod-BSA complexes are CDS inactive and that Au nanorod dimers, trimers, and larger aggregates complexes show structure-dependent CDS. In other work, we focused on exploring the plasmonic effect on superlocalization of fluorescent dyes in single- molecule studies. We present a fitting method for abnormal PSFs using a basis of Hermite-Gaussian functions and show that orientation information is encoded in bi-lobed PSFs. A third project focused on protein unfolding behaviors and the effect from surrounding environment using single-molecule high- resolution imaging with photobleaching (SHRIMP) to resolve conformational changes of multi-dye- labeled proteins.

L-E-0001, ENDOWMENT IN CHEMISTRY AND RELATED SCIENCES (TcSUH), University of Houston.

The Chen group has discovered several new anode materials for SIBs. Bi₂Se₃ and Sb₂Te₃ are both alloying type of anode materials. They have high capacity but low stability due to large volume change during charging/discharging. Chen's group found that both Bi₂Se₃-carbon composite and Sb₂Te₃-carbon composite can be facilely prepared with a high energy ball milling (HEBM) method. In both materials, Bi₂Se₃ and Sb₂Te₃ particles with a size of about 20 nm embedded in the carbon matrix are produced by HEBM. During charging and discharging, the synergetic effects of carbon matrix and nanosized particles can release stress efficiently and result in high capacity and stable performance. Another SIB anode material is K₂Ti₆O₁₃ nanowires (KTO). KTO exhibits a tunnel structure and is favorable for sodium ion intercalation. In addition, the average operating voltage of K₂Ti₆O₁₃ is about 0.7 V vs. Na⁺/Na. Therefore, KTO could potentially be a safe and high performance anode material. However, pristine KTO has low electrical conductivity and poor rate

capability. In this work, highly conductive black K₂Ti₆O₁₃ (B-KTO) nanowires are synthesized. The B-KTO nanowires have diameters of 6-10 nm and lengths up to 3 μm. The B-KTO electrode delivers a high capacity and no obvious capacity fading after 20,000 cycles in a half cell.

For water electrolysis to produce hydrogen gas, phosphide-based materials, such as Ni/Ni₅P₄/NiP₂, FeP/Ni₂P, and CoP/Ni₅P₄/CoP anchored on porous nickel foams were developed by the Chen group. The materials are synthesized by direct phosphorization of nickel foams, which ensures excellent electrical contact, low overpotential, and high durability. For example, CoP/Ni₅P₄/CoP requires an overpotential of only 33 mV to achieve the benchmark 10 mA cm⁻² for hydrogen evolution reaction (HER), which is superior to most electrocatalysts made of metal phosphides, and performs comparably to the state-of-the-art Pt catalysts.

H-C-0034, EQUIPMENT PURCHASES, Rice University.

There were no expenditures from the Welch Foundation Equipment Grant in 2017-2018. These funds will be used as needed for equipment purchases for Dr. George Phillips in the Department of Biosciences and for Dr. Peter Wolynes and Dr. K.C. Nicolaou in the Department of Chemistry. Since their recruitment to Rice, these faculty members have established prominent research programs and become vital members of the academic community.

The overall goal of the research in Dr. Phillips's laboratory is to relate the three-dimensional structure and dynamics of proteins to their biological functions. His lab uses techniques of X-ray crystallography and other biophysical methods to elucidate the molecular structures, dynamics, and functions of proteins. Extensive use is made of modern computational methods to analyze the structures and their dynamics.

Research in Dr. Wolynes's laboratory is broadly concerned with many-body phenomena in biology, chemistry, and physics. A major theme is understanding systems where a large diversity of long lived states is involved, necessitating the use of a statistical characterization of an energy or attractor landscape. The most notable examples are glasses, liquids, biomolecules and biomolecular regulatory networks.

Dr. Nicolaou's research focuses on the advancement of organic synthesis for its own sake and its application to the synthesis of natural and designed molecules of biological and medical importance. Current projects in the group include the total synthesis of highly potent and scarce naturally occurring cytotoxic molecules and their analogues as payloads for antibody-drug conjugates (ADCs) for targeted personalized cancer therapies.

The Welch Foundation's support will allow these faculty members the flexibility to make further equipment purchases in support of the continued development of their respective research programs. We are grateful for the Welch Foundation's meaningful investment in equipment, which plays a crucial role in research particularly at the nanometer scale, which requires modern, often complex instrumentation. We look forward to providing future updates as funds are expended from the grant.

H-E-0041, CENTER OF EXCELLENCE IN POLYMER CHEMISTRY, University of Houston.

Due to the generous funding of The Robert A. Welch Foundation of \$4,000,000 in 2013, the University of Houston embarked on establishing one of the nation's best centers for polymer chemistry research. Renovations to UH's Center for Excellence in Polymer Chemistry's (CEPC) physical home were completed in 2016. In 2017, after a robust national search, Dr. Eva Harth of Vanderbilt University was named Founding Director of the CEPC. In 2018, the Founding Director established the Harth Laboratory in the College of Natural Sciences and Mathematics.

"Throughout the years, the Welch Foundation has been incredibly generous to the University of Houston," said Dan E. Wells, Dean of the College of Natural Sciences and Mathematics. "We are grateful to receive this grant that will advance our Tier One research and generate a uniquely skilled workforce for Houston and Texas." Chemists develop polymers that can be used to make products for the fiber, communication, packaging and other industries. UH faculty will emphasize fundamental chemistry research, but they also will work with area petrochemical companies seeking to convert natural gas feedstock into advanced materials.

Mike Harold, Chairman of the Department of Chemical Engineering, whose faculty is also involved in the new center, said the gift will speed efforts to develop new polymer products and technologies. "This is especially timely with the domestic energy revolution we are experiencing, since the main feedstocks of polymers are petroleum and natural gas," he said.

David Hoffman, Chairman of the Department of Chemistry, said the money will do more than simply establish a research center. "The Foundation's grant will help the University more rapidly expand and enhance its research on polymers, an area of research important to Texas and, in particular, Houston because of its close proximity and ties to the petrochemical industry," Hoffman said.

H-F-0001, WELCH SUMMER SCHOLARS PROGRAM. The University of Texas at Austin.

On behalf of the site directors and the high school students who were supported by the 2017 Welch Summer Scholars Program, I am happy to report the successful completion of the 2017 WSSP. This past summer, 41 talented and energetic Texas high school students were hosted at the five WSSP sites. The scientific accomplishments of these students during the summer have already been forwarded to The Welch Foundation in the WSSP 2017 Research Book.

Our 2017 cohort of Scholars participated in a broad spectrum of basic research in chemical synthesis, chemical biology, biophysics, analytical chemistry, materials science, and computational modeling. During the five-week program, these students gained meaningful experience in authentic research while learning chemical safety and hygiene; respect for laboratory and environmental resources; data collection and management; and effective communication skills. Our site directors also focused on building a strong community of "Welchies" at each location, and consistent feedback from Scholars reveals that the experience of living on a college campus away from home and family is just as important for their personal growth as the laboratory research itself. Comments from these Scholars from our survey at the end of the program are uniformly glowing:

As a Welch Summer Scholar of 2017, I feel that I achieved an incredible balance of summer recreation and laboratory work that contributed significantly to my development as a student and as an individual. (UT-Austin)

Welch was an amazing experience for me. Overall, this experience was the perfect combination of research and enjoyment. If I was invited to participate another year, I wouldn't blink twice before saying yes. (UT Dallas)

I never imagined I would be able to work closely with grad students, post docs, or professors before entering college, but the Welch program let me do just that. I got first-hand experience of how unpredictable yet rewarding studying and working in the science field is. I have also made some great friends of the course of the program through fun movie nights and talking about our research. I am thankful I was able to partake in this program! (University of Houston)

There were several new developments throughout the year:

1) Brenda Baxendale was hired as program coordinator in January 2016. Brenda works with me at UT-Austin in all aspects of program advertising and recruitment, Scholar selection, and program management for all five WSSP sites.

2) We have begun working with Michaela Williams and Mary Ann Cuellar at Dancie Perugini Ware Public Relations to raise the public profile of the WSSP. We have had meetings in person and by phone with Michaela and Mary Ann to educate them about the program and brainstorm how we can work together for our mutual benefit. We have supplied them with WSSP-related content for the Welch Foundation Facebook page and we will be working with them over the coming year to improve our alumni network.

3) We have made progress towards our goals of expanding our applicant pool to include applications from areas of the state that have been traditionally underrepresented in the WSSP community, including from Laredo and the Rio Grande valley. We have been working with ChemBridge, a high school dual credit program focused on school districts that are underrepresented at UT-Austin, and are making contacts with teachers and councilors at these schools. We had one applicant from a ChemBridge school last year, and we are working to increase that number this year.

I look forward to another successful year in 2018. Thank you for The Welch Foundation's continued support of the WSSP.

H-F-0037, TEXAS CENTER FOR ELECTROCHEMISTRY, The University of Texas at Austin.

Using this grant, the CEC SUPPORTED, (A) an annual CEC Workshop on electrochemistry and (B) an electrochemical research instrumentation facility.

A. 2018 CEC Annual Workshop on Electrochemistry: The annual workshop was organized and run by the CEC and took place on February 10–11, 2018 on the UT-Austin campus. There were 160 registered attendees for this conference, which brought together experts from academia, industry, and national laboratories. This year's meeting format featured four dedicated sessions: Electrochemistry for the Climate and Environment, Next Generation Batteries, and In situ Characterization of Intermediates in Electrocatalysis. The meeting also included a robust poster session in which students, postdocs, and researchers from universities, national labs, and industry presented 37 posters and answered questions from attendees in an informal evening session. An expo featuring electrochemical instrumentation from some of the CEC industrial Affiliates accompanied the poster session. Students and postdocs also enjoyed informal discussions with invited speakers over lunch.

B. Electrochemical Research Instrumentation Facility: For the current reporting period, the CEC continued to maintain and operate a unique facility for electrochemical research for scientists in Texas that allows them to have access to facilities and expert help in electrochemical studies. The CEC facility complements extensive facilities available at UT-Austin (such as the TMD). This facility is used by CEC research groups and affiliates and is available as a user facility for other Texas universities and colleges. Dr. Joy Chen is employed as a full-time staff member to maintain the facility and assist visitors.

H-K-0029, THE ACADEMY OF MEDICINE, ENGINEERING AND SCIENCE OF TEXAS.

TAMEST's 2019 Annual Conference will explore the groundbreaking research that could lead to advances in neuroscience and better brain health. It will investigate topics such as healthy aging, addiction and the opioid crisis, neurological disease prevention, technological advances in mapping the brain, and neuroscience research priorities and challenges that lie ahead.

The annual gathering in January of the state's top scientists, industry and community leaders, and university presidents and chancellors is TAMEST's premiere event, providing a forum for sharing information and fostering interdisciplinary collaboration in research efforts across the state. By sponsoring this event, the Welch Foundation ensures Texas' place as a national leader in medicine, science, technology innovation, and economic opportunity.

H-Q-0042, CENTER FOR DRUG DISCOVERY, Baylor College of Medicine.

We thank the Welch Foundation for the first 3 years of funding of our 2015 grant proposal. This award has been fundamental in allowing the Center for Drug Discovery (CDD) at BCM to establish the DNA-encoded chemistry technology (DEC-Tec) platform. In addition to funds from BCM to maintain the CDD, we have leveraged the Welch Foundation funds to bring in additional funds to expand and enhance our operation in this area. These funds are as follows:

1) In June 2016, we were awarded a 5-year \$6 million Core Facility Support Award from CPRIT entitled "Preclinical Candidate Discovery Core." In addition to funds for personnel and supplies, this grant contributed equipment funds for a new mass spectrometer (\$362,864) for our group.

2) We secured \$1 million from the Mabee Foundation and \$4.4 million in matching funds for infrastructure support. These funds were used for building critically needed chemistry space for the CDD on the 6th floor of the Texas Children's Hospital Neurological Research Institute (NRI) (as the Board observed during their recent tour). This 25,000 sq. ft. space (75% built to date) houses 20 chemical fume hoods. Our chemistry group moved into this facility in October 2017. There are several advantages of this location:

A. It is centrally located in the Texas Medical Center (TMC), allowing our drug discovery efforts to be more easily integrated with the wide range of research in the TMC.

B. It places us close to Dr. Huda Zoghbi's operation in the NRI and future Texas Children's Hospital hematology-oncology laboratories.

C. The CDD NMR facility (with 600 MHz and 800 MHz NMRs) is already located on the 2nd floor of the NRI; this NMR facility has been completed.

3) From March 2016-December 2017, we were engaged in a 22-month collaborative contract with a biotech partner. We learned much during the collaboration, and we now are stronger and more equipped to generate DEC-Tec libraries and perform selections independently. This \$4.6 million collaborative relationship allowed the following:

A. Our collaborative partner addressed freedom-to-operate issues in the DNA-encoded chemistry space. The partner would like confidentiality of our agreement at this time, and we have submitted our first manuscript in collaboration with our partner.

B. The partner contributed novel scaffolds and large collections of unique building blocks for the synthesis of innovative DEC-Tec libraries at BCM.

C. The partner contributed two unique DEC-Tec libraries for screening at BCM and also is receiving 50% of each DEC-Tec library produced at BCM. Libraries are synthesized at scales that enable thousands of selection experiments for BCM targets.

D. Our collaborative partner contributed support for personnel and supplies and >\$750,000 toward equipment required to construct and use DEC-Tec libraries.

E. Our biotech partner made significant intellectual contributions in both library design and selection strategies. Our partner employs outstanding scientists with extensive industrial experience using DEC-Tec for drug discovery who have advised BCM scientists on methods to improve BCM DEC-Tec processes.

4) For our research in male contraception, we received Global Grand Challenges Phase I funding from the Gates Foundation for screening of our libraries with male germ cell-specific targets (\$100,000; Nov 1, 2016 – Oct 31, 2018); we are preparing our Phase 2 application now (due November 2018). Our NIH program project (P01) grant entitled "Functional genomics and DEC-Tec to identify germ cell-specific contraceptives" received a 1% score and started May 1, 2017. The awarded 5-year P01 budget is \$6.19 M (direct and indirect costs).

PUBLICATIONS BY PRINCIPAL INVESTIGATORS REPORTED DURING 2017 – 2018*

Research Grants.....	121
Endowed Chairs	205
Departmental Grants.....	224
Other Endowed Grants	228

*The publication listings recorded in this annual report supplement are published exactly as they were submitted.

RESEARCH GRANTS

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