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THE ROBERT A. WELCH FOUNDATION
58TH CONFERENCE ON CHEMICAL RESEARCH
“CHEMICAL EDUCATION”

Monday, October 27, 2014

- 8:30 **WILHELMINA E. ROBERTSON**, Chair of the Board of Directors
8:35 **MARYE ANNE FOX**, University of California, San Diego, Program Chair

SESSION I -

- 8:40 **DUDLEY R. HERSCHBACH**, Texas A&M University & Harvard University, Discussion Leader
- 8:50 **LARRY R. FAULKNER**, The University of Texas at Austin,
“Advancing Graduate Education in the Chemical Sciences”
Discussion
- 9:40 **BRUCE ALBERTS**, University of California, San Francisco,
“Spreading a Scientific Spirit Throughout Society: Why and How?”
Discussion
- 10:30 Break
- 10:45 **CARL WIEMAN**, Stanford University,
“Taking a Scientific Approach to Science Education”
Discussion
- 11:35 **ERIC MAZUR**, Harvard University,
“Assessment: The Silent Killer of Learning”
Discussion
- 12:25 LUNCH

SESSION II

- 1:30 **KEITH J. STEVENSON**, University of Texas at Austin, Discussion Leader
- 1:40 **ISIAH M. WARNER**, Louisiana State University,
“LA-STEM Research Scholars Program: A Model for Broadening Diversity and Participation in STEM”
Discussion
- 2:30 **BASSAM Z. SHAKHASHIRI**, University of Wisconsin-Madison,
“Enlightenment and the Responsibilities of the Enlightened”
Discussion
- 3:20 **RICHARD TAPIA**, Rice University,
“Crisis in Representation in Higher Education: A Need for New Understanding and New Leadership”
Discussion
- 4:10 Adjourn

Tuesday, October 28, 2014

SESSION III

- 8:00 **MAHA ZEWAİL-FOOTE**, Southwestern University, Discussion Leader
- 8:10 **MICHAEL P. MARDER**, The University of Texas at Austin (UTeach),
 "Preparing Science and Mathematics Teachers at Universities with UTeach"
 Discussion
- 9:00 **BRIAN P. COPPOLA**, University of Michigan,
 "Lessons from Three Decades of Subversion"
 Discussion
- 9:50 Break
- 10:05 **JOHN ARNOLD**, University of California, Berkeley,
 "Greening the Chemistry Curriculum"
 Discussion

2014 Welch Awardee Lecture

- 10:55 **ROBERT G. BERGMAN**, University of California, Berkeley,
 "Selective Stoichiometric and Catalytic Reactions in Water Soluble Host-Guest Supramolecular Systems"
- 11:35 LUNCH

SESSION IV

- 1:00 **MARCY H. TOWNS**, Purdue University, Discussion Leader
- 1:10 **ANANT AGARWAL**, edX, (via webex)
 "Reinventing Education"
 Discussion
- 2:00 Break
- 2:15 **ARTHUR B. ELLIS**, City University of Hong Kong,
 "The City University Discovery-Enriched Curriculum"
 Discussion
- 3:05 **SALLY M. JOHNSTONE**, Western Governor's University,
 "How Competency-Based Education Fits for Chemistry Education"
 Discussion
- 3:55 Adjourn

**THE ROBERT A. WELCH FOUNDATION
CONFERENCES ON CHEMICAL RESEARCH
1957 – 2013**

<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

**WELCH AWARD RECIPIENTS
1972 - 2013**

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

HACKERMAN AWARD RECIPIENTS

2002 - 2014

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

PRINCIPAL INVESTIGATORS

2013 - 2014

Abanov	Artem G.	A-1678	Chen	Zheng	AU-1731
Addo-Mensha	Alfred K.	BS-1779	Chen	Zhijian J.	I-1389
Ahn	Jung-Mo	AT-1595	Chiang	Cheng-Ming	I-1805
Alper	Hal S.	F-1753	Chiu	Wah	Q-1242
Alto	Neal M.	I-1704	Chook	Yuh Min	I-1532
Altschuler	Steven J.	I-1619	Chuang	David T.	I-1286
Alu	Andrea	F-1802	Chung	Yeonseok	L-AU-0002
An	Zhiqiang	AU-0042	Clearfield	Abraham	A-0673
Anslyn	Eric V.	F-1151	Clementi	Cecilia	C-1570
Armstrong	Daniel W.	Y-0026	Cobb	Melanie H.	I-1243
Atassi	M. Zouhair	Q-0007	Coffer	Jeffery L.	P-1212
Balakotaiah	Vemuri	E-1152	Coltart	Don M.	E-1806
Baldelli	Steven	E-1531	Conrad	Nicholas K.	I-1732
Balkus, Jr.	Kenneth J.	AT-1153	Contreras	Lydia M.	F-1756
Ball	Zachary	C-1680	Corey	David R.	I-1244
Bankaitis	Vytas A.	BE-0017	Cowley	Alan H.	F-0003
Bao	Jiming	E-1728	Crooks	Richard M.	F-0032
Bard	Allen J.	F-0021	Cuello	Luis G.	BI-1757
Barondeau	David P.	A-1647	Dalby	Kevin N.	F-1390
Barrick	Jeffrey E.	F-1780	Darensbourg	Donald J.	A-0923
Barron	Andrew R.	C-0002	Darensbourg	Marcetta Y.	A-0924
Bartel	Bonnie	C-1309	Daugulis	Olafs	E-1571
Baughman	Ray H.	AT-0029	De Brabander	Jef K.	I-1422
Begley	Tadhg P.	A-0034	Deberardinis	Ralph J.	I-1733
Belkin	Mikahil A.	F-1705	DeMartino	George N.	I-1500
Benedek	Nicole A.	F-1803	Dias	H. V. Rasika	Y-1289
Bennett	Matthew R.	C-1729	Diehl	Michael R.	C-1625
Bergbreiter	David E.	A-0639	Dong	Guangbin	F-1781
Bernal	Ricardo A.	AH-1649	D'Orso	Ivan	I-1782
Bevan	John W.	A-0747	Downer	Michael	F-1038
Bezprozvanny	Ilya B.	I-1754	Drezek	Rebekah	C-1598
Billups	W. E.	C-0490	Du	Rui-Rui	C-1682
Birney	David M.	D-1239	Dunbar	Kim R.	A-1449
Biswal	Sibani, L.	C-1755	Dunning	F. Barry	C-0734
Bittner	Eric R.	E-1337	Echegoyen	Luis	AH-0033
Blount	Paul	I-1420	Elber	Ron	F-1783
Bluemel	Janet	A-1706	Ellington	Andrew D.	F-1654
Borden	Weston T.	B-0027	Ellison	Christopher J.	F-1709
Brodbelt	Jennifer S.	F-1155	Estreicher	Stefan K.	D-1126
Brown	Kathlynn C.	I-1622	Falck	J. Russell	I-0011
Bruick	Richard K.	I-1568	Fan	Donglei L.	F-1734
Burgess	Kevin	A-1121	Fast	Walter	F-1572
Burgess	Shawn C.	I-1804	Findlater	Michael	D-1807
Chapman	Walter G.	C-1241	Finkelstein	Ilya J.	F-1808
Chen	Banglin	AX-1730	Fitzpatrick	Paul F.	A-1245
Chen	Chuo	I-1596	Folden, III	Charles M.	A-1710

PRINCIPAL INVESTIGATORS
2013 - 2014

Foster	Matthew S.	C-1809	Jayaram	Makkuni	F-1274
Frantz	Doug E.	AX-1735	Jiang	Jean X.	AQ-1507
Futreal	Andrew	G-0040	Jiang	Jin	I-1603
Gabbaï	François P.	A-1423	Jiang	Ning	F-1785
Ganesan	Venkat	F-1599	Jiang	Qui-Xing	I-1684
Gardner	Kevin H.	I-1424	Jiang	Youxing	I-1578
Garner	Charles M.	AA-1395	Jianping	Jin	AU-1711
Garrard	William T.	I-0823	Johnson	Kenneth A.	F-1604
Gladysz	John A.	A-1656	Johnston	Keith P.	F-1319
Glasner	Margaret E.	A-1758	Jones	Richard A.	F-0816
Gohil	Vishal M.	A-1810	Kadish	Karl M.	E-0680
Golding	Ido	Q-1758	Kaplan	Craig D.	A-1763
Goldsmith	Elizabeth J.	I-1128	Keatinge-Clay	Adrian T.	F-1712
Goodenough	John B.	F-1066	Kelly	Kevin F.	C-1605
Gorenstein	David G.	AU-1296	Kerwin	Sean M.	F-1298
Green	Kayla N.	P-1760	Kiang	Ching-Hwa	C-1632
Grigolini	Paolo	B-1577	Kim	Chongwoo A.	AQ-1813
Grishin	Nick V.	I-1505	Kim	Tae-Kyung	I-1786
Guloy	Arnold M.	E-1297	Klein	Douglas J.	BD-0894
Gurha	Priyatansh	L-AU-0002	Klein	William H.	G-0010
Gustafsson	Jan-Åke	E-0004	Kliewer	Steven	I-1558
Hafner	Jason H.	C-1761	Ko	Che Ming	A-1358
Halas	Naomi J.	C-1220	Kohler	Jennifer J.	I-1686
Halasyamani	P. Shiv	E-1457	Kolomeisky	Anatoly B.	C-1559
Hall	Michael B.	A-0648	Kono	Junichiro	C-1509
Hanna	Tracy A.	P-1737	Korgel	Brian A.	F-1464
Hardy	John C.	A-1397	Kouri	Donald J.	E-0608
Harshey	Raskia M.	F-1811	Krische	Michael J.	F-0038
Hart	P. John	AQ-1399	Kürti	László	I-1764
Hartgerink	Jeffrey D.	C-1557	Laane	Jaan	A-0396
Hase	William L.	D-0005	Lai	Keji	F-1814
Heller	Adam	F-1131	Lambert	David L.	F-0634
Hibbs	Ryan E.	I-1812	Lambowitz	Alan M.	F-1607
Hiesinger	Peter R.	I-1657	Landes	Christy F.	C-1787
Hilty	Christian B.	A-1658	Larionov	Oleg V.	AX-1788
Hoffman	David M.	E-1206	Lee	James C.	H-0013
Holliday	Bradley J.	F-1631	Lee	Seongmin	F-1741
Hooper	Lora V.	I-1762	Lee	T. Randall	E-1320
Hsieh	Jenny	I-1660	Lei	Xiangyang	V-1815
Huang	Huey W.	C-0991	Li	Bing	I-1713
Hulet	Randall G.	C-1133	Li	Guigen	D-1361
Humphery	Simon B.	F-1738	Li	Pingwei	A-1816
Hwang	Gyeong S.	F-1535	Li	Xiaoqin (Elaine)	F-1662
Igumenova	Tatyana I.	A-1784	Lichti	Roger L.	D-1321
Iverson	Brent L.	F-1188	Lindahl	Paul A.	A-1170
Jacobson	Allan J.	E-0024	Link	Stephan	C-1664

PRINCIPAL INVESTIGATORS

2013 - 2014

Liou	Jen	I-1789	Niu	Qian	F-1255
Liu	Hung-wen	F-1511	Nordlander	Peter J.A.	C-1222
Liu	Jun	AU-1714	North	Simon W.	A-1405
Liu	Qinghau	I-1608	Olson	Eric N.	I-0025
Liu	Wenshe	A-1715	Olson	John S.	C-0612
Liu	Xin	I-1790	Omary	Mohammad A.	B-1542
Liu	Yi	I-1560	Onuchic	José	C-1792
Lockless	Steve W.	A-1742	Orth	Kim	I-1561
Lou	Jun	C-1716	Ozerov	Oleg V.	A-1717
Lovely	Carl J.	Y-1362	Pannell	Keith H.	AH-0546
Lubchenko	Vassiliy	E-1765	Pasare	Chandrashekar	I-1820
Lucchese	Robert R.	A-1020	Pasquali	Matteo	C-1668
Lum	Lawrence	I-1665	Pellois	Jean-Philippe	A-1769
Lutkenhaus	Jodie L.	A-1766	Pettitt	B. Montgomery	H-0037
Lyuksyutov	Igor	A-1688	Phillips	Margaret A.	I-1257
Ma	Jianpeng	Q-1512	Poirier	Lionel W.	D-1523
MacDonald	Allan H.	F-1473	Potts	Patrick Ryan	I-1821
MacDonnell	Frederick M.	Y-1301	Prasad	B. V. Venkataram	Q-1279
MacMillian	John B.	I-1689	Prokai	Laszlo	BK-0031
Magnus	Philip D.	F-0018	Pu	Han	C-1669
Makarov	Dmitrii E.	F-1514	Quiococho	Florante A.	Q-0581
Mangelsdorf	David J.	I-1275	Radhakrishnan	Arun	I-1793
Manjavacas	Alejandro	L-C-0004	Raizen	Mark G.	F-1258
Manthiram	Arumugam	F-1254	Ranganathan	Raman	I-1366
Marcotte	Edward M.	F-1515	Rao	Hai	AQ-1747
Markert	John T.	F-1191	Rauschel	Frank M.	A-0840
Marshall	Paul	B-1174	Ray	Asok K.	Y-1525
Marti-Arbona	Angel A.	C-1743	Ready	Joseph M.	I-1612
Martin	Stephen F.	F-0652	Reichl	Linda E.	F-1051
Masters	Bettie Sue	AQ-0012	Ren	Pengyu	F-1691
Matouschek	Andreas	F-1817	Richmond	Michael G.	B-1093
Matsuda	Seiichi P.T.	C-1323	Rimer	Jeffrey D.	E-1794
Matthews	Kathleen S.	C-0576	Rizo-Rey	Jose	I-1304
May	Jeremy A.	E-1744	Robertus	Jon D.	F-1225
Maynard	Jennifer A.	F-1767	Romo	Daniel	A-1280
Miljanic	Ognjen Š.	E-1768	Rose	Michael J.	F-1822
Mills	Nancy S.	W-0794	Rosen	Michael K.	I-1544
Moore	David D.	Q-0022	Rosenbaum	Daniel M.	I-1770
Morosan	Emilia	C-1791	Ross, Jr.	Joseph H.	A-1526
Mullins	Charles B.	F-1436	Rosky	Peter J.	F-0019
Musser	Siegfried	BE-1541	Russell	Rick	F-1563
Natelson	Douglas	C-1636	Sacchetti	James C.	A-0015
Natowitz	Joseph B.	A-0330	Schmid	Sandra L.	I-1823
Naugle	Donald G.	A-0514	Scholtz	J. Martin	BE-1281
Nevidomskyy	Andriy	C-1818	Schuessler	Hans A.	A-1546
Nicolaou	Kyriacos C.	C-1819	Scully	Marlan O.	A-1261

PRINCIPAL INVESTIGATORS
2013 - 2014

Scuseria	Gustavo E.	C-0036	Wang	Zhigao	I-1827
Segatori	Laura	C-1824	Watanabe	Coran	A-1828
Serwer	Philip	AQ-0764	Webb	Lauren J.	F-1722
Sessler	Jonathan L.	F-1018	Weinberg	Steven	F-0014
Shan	Libo	A-1795	Weisman	R. Bruce	C-0807
Shear	Jason B.	F-1331	Wensel	Theodore G.	Q-0035
Sherry	A. Dean	AT-0584	Westover	Kenneth D.	I-1829
Shi	Xioabing	G-1719	Wheeler	Steven E.	A-1775
Shih	Chih-Kang	F-1672	White	Michael A.	I-1414
Shin	Ok-Ho	H-1771	Whitman	Christian P.	F-1334
Si	Qimiao	C-1411	Whitmire	Kenton H.	C-0976
Siegel	Dionicio R.	F-1694	Willets	Katherine A.	F-1699
Silberg	Jonathan J.	C-1614	Willson	Richard C.	E-1264
Simanek	Eric E.	P-0008	Wilson	Lon J.	C-0627
Smith, Jr.	Dennis W.	AT-0041	Wolynes	Peter G.	C-0016
Sokolov	Alexei V.	A-1547	Wood	John L.	AA-0006
Son	Dong Hee	A-1639	Wooley	Karen L.	A-0001
Songyang	Zhou	Q-1673	Wu	Lani F.	I-1644
Spudich	John L.	AU-0009	Wyatt	Robert E.	F-0362
Stanton	John F.	F-1283	Yacaman	Miguel Jose	AX-1615
Stefan	Mihaela C.	AT-1740	Yakobson	Boris I.	C-1590
Stevenson	Keith J.	F-1529	Yan	Nan	I-1831
Stocco	Douglas M.	BI-0028	Yang	Ding-Shyue	L-E-0001
Straight	Paul D.	A-1796	Yang	Jiong	A-1700
Su	Wu-Pei	E-1070	Yao	Yan	L-E-0001
Tambar	Uttam K.	I-1748	Yarovinsky	Felix	I-1799
Tao	Yizhi Jane	C-1565	Ye	Jin	I-1832
Terman	Jonathan R.	I-1749	Yeager	Danny L.	A-0770
Thomann	Isabell	C-1825	Yeh	Hsin-Chih	F-1833
Thummel	Randolph P.	E-0621	Yennello	Sherry J.	A-1266
Ting	Chin-Sen	E-1146	Yeo	Hye-Jeong	E-1616
Tittel	Frank K.	C-0586	Yu	Gang	I-1776
Tonzetich	Zachary J.	AX-1772	Yu	Hongtao	I-1441
Truskett	Thomas M.	F-1696	Yu	Yonghao	I-1800
Tsai	Francis T.F.	Q-1530	Zakhidov	Anvar A.	AT-1617
Tu	Benjamin P.	I-1797	Zhang	Chengcheng	I-1834
Urbach	Adam R.	W-1640	Zhang	Chun-Li	I-1724
Uyeda	Kosaku	I-1720	Zhang	Renyi	A-1417
Van Hoof	Ambro	AU-1773	Zhang	Xiuren	A-1777
Varadarajan	Navin	E-1774	Zhang	Xuewu	I-1702
Walker	Cheryl Lyn	BE-0023	Zhang	Yan Jessie	F-1778
Wan	Yihong	I-1751	Zhao	John C.-G.	AX-1593
Wang	Dachun	L-AU-0002	Zheltikov	Aleksei M.	A-1801
Wang	Jin	Q-1798	Zheng	Junrong	C-1752
Wang	Qinghua	Q-1829	Zhou	Hongcai Joe	A-1725
Wang	Yuhong	E-1721	Zhu	Xiaoyang	F-1726

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.

ARTEM G. ABANOV, A-1678, Texas A&M University. QUANTUM COHERENT SYNTHESIS AND DECOMPOSITION.

I continued to study the diatomic molecular coherent formation reaction at ultra low temperatures. At such conditions the quantum coherent nature of the atoms and the quantum coherence in between the collisions cannot be ignored. Moreover, as the temperature is ultra low, and the energy must be conserved the reaction may happen only at the conditions close to the resonance between the state of two separate atoms and the ground state of the formed molecule. Such resonance conditions may be achieved by bringing the gas of atoms to the vicinity of Feshbach resonance by an external magnetic field. At the resonance one has to consider the coherence between the state of the interacting atoms and molecules. The relevant length scale in the system - the scattering length - diverges at the resonance. The resulting multiparticle state must be a new universal macroscopic quantum mechanical state. At the present stage of the research my students and I are trying to find the quantum mechanical ground state wave function and its properties of such a system. The wave function must be universal, scale invariant, and rigid. In this sense it should not depend on the details of the Hamiltonian. The approach we have employed is to find a simple Hamiltonian which have the desired properties and investigate the multiparticle ground state wave function of such a Hamiltonian

ALFRED K. ADDO-MENSHA, BS-1779, Texas A&M International University. THE DESIGN, SYNTHESIS, CHARACTERIZATION AND BINDING STUDIES OF MULTIVALENT POLYPRIDINE BASED MACROCYCLIC CARBOHYDRATE RECEPTORS IN AQUEOUS SOLUTIONS.

This year was a buildup on the previous year. The monomeric receptor has been successfully synthesized and a protocol for purification has been developed and currently being validated. The peptide has been synthesized and currently the linking of the monomer and peptide is under development. Results of solid phase synthetic routes that were successful were published in an undergraduate honor's thesis by one of the students. Also, initial titrations of monomer with selected monosaccharides were presented at a local conference and the source of funding was rightly acknowledged. The PI is currently waiting for a final approval for software needed to calculate thermodynamic parameters. This grant was very instrumental in helping the PI obtain two grants from NSF to purchase NMR and PS3 Peptide Synthesizer which have been successfully installed. These instruments will help in the synthesis of the receptors and in the characterization process.

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

In this third grant year, we have focused on improving the leading compounds that were synthesized and identified in the previous year. As the LXXLL motif plays a critical role in protein-protein interactions mediated by nuclear receptors like androgen receptor (AR), we have designed and synthesized bis-benzamides that can reproduce one-side of helical protein surfaces by presenting two side chain functional groups located at the *i* and *i+4* positions of the helical motif. The resulting bis-benzamides demonstrated outstanding inhibitory activities on many prostate cancer cell lines, such as disruption of AR-coactivator complexes, inhibition of AR nuclear translocation, inhibition of AR-mediated gene transcription, and inhibition of AR-mediated cell proliferation. These results were summarized and published in *Nature Communications* in 2013. To improve the LXXLL motif-mimicking bis-benzamides, we have introduced additional functional groups to the leading bis-benzamides based on the flanking sequences near the LXXLL core. We have synthesized about thirty tris-benzamides and evaluated them on AR-positive prostate cell lines like LNCaP and LAPC4. It is exciting that several tris-benzamides showed comparable or higher cell growth inhibition and they are currently under further evaluation *in vitro* and *in vivo*. We have also tested our bis- and tris-benzamides on breast cancer cell lines as estrogen receptor also uses the LXXLL motif to recruit its coactivators. These oligo-benzamides remarkably showed strong growth inhibition of breast cancer cell lines, suggesting a potential of oligo-benzamides in treating breast cancer as well as prostate cancer.

HAL S. ALPER, F-1753, The University of Texas at Austin. A SYNTHETIC BIOCHEMISTRY PLATFORM FOR ALKANE SYNTHESIS IN YEAST.

Last grant year, we engineered a pentane production pathway. In this grant year, we have introduced synthetic metabolic pathways to enable high-chain alkane synthesis and diversification. Through the incorporation of a thioesterase into our engineered strain, we have been able to produce mg/L quantities of various fatty acids including Caprylic acid (C8:0), Capric Acid (C10:0), Lauric Acid (C12:0), and Myristic Acid (C14:0). Through the introduction of modifying enzymes, we have been able to produce diversified products such as vernolic acid and ricinoleic acid. Moreover, through the introduction of a fatty acid reductase and a fatty aldehyde decarbonylase based pathway, we have been able to demonstrate at the mass-spectrometry level, the presence of alkane products from the various fatty acids produced.

Additionally this year, we further engineered our strain of *Y. lipolytica* through an evolutionary engineering approach. This strain is now capable of producing upwards of 40 g/L of lipids in a bioreactor condition (compared to 25 g/L in our prior strain engineered during last grant year). This strain now serves as a host for producing high levels of diversified oleochemicals, the subject of our renewal Welch Grant.

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

We have proposed to determine the molecular and structural basis of action of the Invasion plasmid antigen J (IpaJ), a novel *Shigella* virulence factor with a currently unknown enzymatic and host cellular function. In the previous funding year, we reported for the first time that IpaJ is a cysteine protease that cleaves the N-myristoyl lipid modification from human signaling enzymes including ARE GTPase, Src kinase, and MARCKS (*Nature*, 2013). Protein N-myristoylation is essential for both viral and parasitic infection as well as oncogene function and therefore our discovery of a protein "demyristoylase" secreted by a bacterial pathogen opens up entirely new avenues in infectious disease and cancer research. We are now working on the X-ray

crystal structure of IpaJ in complex with lipid modified substrates (Specific Aim 2) to address these important issues. We have made significant progress on these goals. Importantly, we have established an *in vitro* protease reaction system that has allowed us to define the molecular mechanism of lipid-dependent proteolysis and to define the minimal-stable protein regions of IpaJ necessary for future structural studies. In addition, we have established collaboration with Dr. Howard Hang (Rockefeller University) to couple state-of-the-art click chemistry procedures (based Azide alkyne Huisgen cycloaddition) with mass spectrometry to screen the human "Myristoylome" for physiological targets of IpaJ. Finally, we have determined how a functional analog of IpaJ, called EspG, selectively inhibits cargo transport through the human ER and Golgi apparatus. Because we have fully reconstituted this pathogenic process *in vitro*, this work was recently published in the Cell press journal *Cell Reports* (2014). Our future work is now aimed at structural determination of IpaJ in complex with host lipidated substrates and also to define mechanisms that drive bacterial and host lipid interactions (Submitted Manuscripts).

STEVEN J. ALTSCHULER, I-1619, The University of Texas Southwestern Medical Center. MECHANISM AND ZONATION OF HEPATIC CROSSTALK LIPOGENESIS AND CANONICAL Wnt-SIGNALING.

In the past year of this grant funding, we focused on investigating cross-pathway interactions among Wnt/ β -catenin, TGF β and BMP signaling pathways. First, these pathways provide highly-studied systems for understanding how cells process morphogenic signals. Second, these pathways are deeply conserved across metazoans, are essential to development, and frequently coordinate cell-fate decisions within tissue compartments. Third, these pathways provide two interesting and contrasting case studies for pathway integration. As classically defined, the Wnt/ β -catenin and TGF β pathways do not share core signaling components; it is difficult to predict whether these pathways interact during transduction, though a number of studies have identified putative interactions. In contrast, the paralogous TGF β and BMP pathways do share a core signaling component (Smad4); competition for this shared component suggests inhibitory crosstalk between these pathways. Fourth, the three pathways co-regulate multiple target genes at the level of transcription. Finally, while the Wnt/ β -catenin, TGF β , and BMP pathways have been studied for decades, they have been less studied in combination and, to date, combinatorial studies have primarily revealed context-specific behaviors.

For crosstalk between the Wnt/ β -catenin and TGF β pathways, we stimulated cells with combinations of signaling of recombinant Wnt3A and TGF β 3, and subsequently monitored whether nuclear β -catenin and Smad2/3 signaling or Axin250 and Smad76 transcriptional responses are modulated. We measured these cellular responses at short time scales (one to two hours) to minimize the potential for alteration of signaling components due to transcriptional feedback. In contrast to studies that have shown increasingly numerous pathway interconnections, we found that Wnt3A/ β -catenin and TGF β 3 signals are instead insulated at the level of signal transduction and are likely integrated primarily during the process of transcription. For the BMP4 and TGF β 3 pathways, we found that BMP4 and TGF β 3 interact either positively or not at all, instead of the expected cross-pathway inhibition due to BMP4 and TGF β 3 competition for Smad4 during signal transduction. Taken together, our results suggest that by disentangling the levels of potential cross-pathway integration (transcription vs. signal transduction) we may more precisely pinpoint where and when cells integrate morphogenic signals to make cellular decisions.

ANDREA ALÙ, F-1802, The University of Texas at Austin. ENHANCED OPTICAL MAGNETISM AND CHIRALITY IN PLASMONIC METAMATERIALS: STRONG MOLECULAR SENSITIVITY AND BROADBAND, GIANT CIRCULAR DICHROISM.

In this first year, we have done significant progress towards our final objective. In a recent experimental paper, we have shown the design, assembly and characterization of relatively complex photonic nanocircuits by accurately positioning a number of metallic and dielectric nanoparticles acting as modular lumped elements. The realized nanoparticle clusters produce the desired spectral response described by simple circuit rules and are shown to be dynamically reconfigurable by modifying the direction or polarization of impinging signals. This work represents an important step towards extending the powerful modular design tools of electronic circuits into nanophotonic systems. Related to this effort, we also discussed how these concepts can be applied to realize strong optical magnetism in metamaterials.

Related to our thrust towards realizing strong circular dichroism and chiral response for biomedical sensing, we have shown theoretically and experimentally giant chiral response in twisted metasurface stacks, and developed a rigorous theory to model and characterize these structures. Lately, we have also experimentally shown their application for molecular sensing. We have put forward some exciting work to realize plasmonic nanodevices for THz wave manipulation, which can bring the concept of optical nanocircuits to a new level, with large impact for communication and sensing devices. Finally, we have been able to characterize and model epitaxially smooth silver layers for the next generation of plasmonic materials, with great interest to reduce the impact of metal losses for the applications mentioned above.

ERIC N. ANSLYN, F-1151, The University of Texas at Austin. HIGH-THROUGHPUT SCREENING (HTS) OF ENANTIOMERIC EXCESS VALUES.

Methods for sensing using optical techniques continue to gain popularity due to the fact that they are rapid and can be multiplexed. This is particularly true with regards to industrial applications, such as methods to monitor the outcome of chemical reactions in the pharmaceutical industry. This Welch grant has focused on the analysis of enantiomeric excess (ee). In this regard, over the past year we have created and published an optical sensing technique for the analysis of the ee values of chiral aldehydes. Our method exploits the rapid condensation of a hydrazine with the aldehyde, making a hydrazone carrying a pyridine ring. The product then creates octahedral complexes around Fe(II), which have absorbance bands that are active in circular dichroism (CD) spectroscopy. The signals in the CD curves will allow for ee analysis. In addition, we have extended our methods of sensing to biological applications, where a method for following the activity of kinases *in vitro* and *in vivo* was created. This assay exploited a set of *in-situ* generated receptors that carry peptides known to bind kinases with well-reported phosphate binding entities. Besides biological applications, we reported a method to detect the

chemical warfare agents known as sulfur mustards. This assay was particularly simple to exploit with real-world samples, and was found to be remarkably selective for detection of sulfur mustards over all other classes of chemical warfare agents. During this same grant period, we published a review article in *Chem. Soc. Rev.*, that covers the basics of the mathematical analyses we exploit in many of our optical sensing methods. Lastly, our group continued to work on the synthesis and testing of various virus inhibitors and antidotes to the biotoxin ricin.

VEMURI BALAKOTAIAH, E-1152, University of Houston. EFFECT OF HETEROGENEITIES ON SPATIOTEMPORAL PATTERNS IN CHEMICAL REACTORS.

One main goal of our work was to determine the effect of heterogeneities either in the reacting medium or catalyst activity or conductivity on stationary and moving temperature and concentration patterns in reacting systems. A second goal was to develop reduced order models or description for these complex systems. We investigated the effect of heterogeneity in porosity or permeability on dissolution patterns in carbonate rocks using HCl. It is found that high heterogeneity causes more branching of the dissolution patterns and leads to high fractal dimension. In parallel work, we have also obtained coarse-grained reduced order models for supported catalysts in which the active material consists of isolated crystallites.

STEVEN BALDELLI, E-1531, University of Houston. STRUCTURE AND ORIENTATION OF ROOM-TEMPERATURE IONIC LIQUIDES AT THE ELECTRIFIED GRAPHENE INTERFACE.

Sum frequency generation (SFG) vibrational spectroscopy and contact angle measurements of the ionic liquid, 1-butyl-3-methylimidazolium dicyanamide [BMIM][DCA] at solid-liquid interfaces are reported. Bare solid single-crystal BaF₂ (111) surface, monolayer graphene-coated BaF₂ (111) surface and a bilayer graphene-coated BaF₂ (111) surface are used as the solid substrates. The SFG results show that only [DCA]⁻ are observed at the BaF₂ (111) surface, while both [BMIM]⁺ and [DCA]⁻ are detected on the graphene coated BaF₂ (111) surface. [DCA]⁻ anions are electro-attracted to the positively charged BaF₂ (111) surface and occupy the first layer at the solid-liquid interface. The graphene coating was then biased as an electrode to adjust the surface charge either positively or negatively. The electric field then organized the IL ions according to the graphene charge and the substrate. This is an example of the doping effect of the substrate.

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

During the most recent funding period on the development of new zeolitic molecular sieve materials we synthesized several new molecular sieves known as metal organic frameworks (MOF). This includes a class of MOFs known as zeolitic imidazolate frameworks (ZIF). The crystal structures were solved for three new ZIF materials including a structure templated by an organometallic complex. We have continued to explore the functionalization of the MOFs and related materials for the binding of small molecules including olefins, nitric oxide and hydrogen sulfide. These materials have been incorporated into nonwoven fiber mats by electrospinning. The MOFs have also been incorporated into membranes and the separation of ethanol and water demonstrated.

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

Our laboratory continues efforts to merge synthetic chemistry with biological tools to create fundamentally solutions to chemical problems. A new tripodal peptide ligand for asymmetric rhodium catalysis was discovered this year using an on-bead, high-throughput ligand discover technique developed in our lab, and reported in *Chem. Sci.* the new ligands discovered in this study are highly selective on solid support, but were poorly selective in solution. A combination of kinetic, spectroscopic, and computational methods were used to shed light on the specific folding and aggregation state benefits of the tripodal ligand and of solid-support anchoring. We have also published a new synthesis of daifachronic acid, a functionally unique nematode hormone with important medical implications, using a combination of metabolic engineering and chemical synthesis methods. By engineering yeast to produce a new sterol with appropriate functional-group handles, we vastly improved upon the best reported synthesis (16 steps) to produce daifachronic acid in 4 synthetic steps in 58% overall yield. This efficient and green synthesis uses H₂, O₂, LiOH and methyl acrylate as the only stoichiometric reagents.

The fundamental reactivity studies made possible by the Welch Foundation allow us to open new areas of investigation. In unpublished work, we have demonstrated the ability to functionalize a natural protein, for the first time, at natural abundance in cell lysate. This accomplishment stands in stark contrast to other approaches, nearly all of which require gene-level recombinant changes to achieve reactivity. We recently discovered new time-gated, fluorogenic reactive pro-fluorophores that improve our imaging capabilities, and have discovered the first Src-family kinase activators that function at biologically relevant (sub-micromolar) concentration.

JIMING BAO, E-1728, University of Houston. UNDERSTANDING NANOCRYSTALLINE CoO AS AN EFFICIENT PHOTOCATALYST FOR SOLAR WATER SPLITTING.

- The water-splitting work is finally published in Nature Nanotechnology after four rounds of rigorous reviews.
- A patent is filed; it is being converted to a regular patent application, which will be submitted by July 5.
- Using monochromatic light we identified that CoO nanocrystals have photocatalytic response to light with wavelength up to 650 nm, below the bandgap of CoO.
- . Discovered that the Co to O ratio in CoO is very important for the photocatalytic activity of CoO nanocrystals.

DAVID P. BARONDEAU, A-1647, Texas A&M University. FLUORESCENT PROBES FOR INTERROGATING Fe-S CLUSTER TRANSFER CHEMISTRY.

Fe-S clusters are essential cofactors for proteins and enzymes found in many critical cellular processes. A conserved set (> 10) of biosynthetic proteins is involved in the synthesis and delivery of [2Fe-2S] and [4Fe-4S] clusters. Defects in these biosynthetic proteins are linked to neurodegenerative and cardiovascular disease. Unfortunately, a lack of useful probes limits research aimed at understanding the mechanisms of Fe-S cluster synthesis and delivery. First, we applied electronic absorbance, circular dichroism, and Mössbauer spectroscopies to reveal details of the Fe-S, cluster assembly reaction on the human Fe-S assembly complex and competing DTT-mediated transfer and mineralization chemistry that have implications for the mechanism and study of Fe-S cluster biosynthesis (*JACS* submission target Aug 1st) Second, we initiated a novel strategy to label Fe-S proteins with fluorescent probes and then use energy transfer-based quenching mechanisms to monitor the kinetics of cluster assembly and transfer. A completed proof of concept study highlights this fluorescent labeling technology by monitoring the unprecedented [2Fe-2S] cluster self-exchange reaction between labeled and unlabeled ferredoxin (*PNAS* submission target Aug 31st) We anticipate these probes will be a great resource for the scientific community, and the results generated with these probes will greatly expand our understanding of the chemistry of the Fe-S cluster biosynthetic pathway with implications in human health and disease.

JEFFREY E. BARRICK, F-1780, The University of Texas at Austin. DISCOVERING FUNCTIONAL NUCLEIC ACID FAMILIES BY DEEP SEQUENCING AND FOLD SAMPLING.

(1) After working with deoxyribozymes with little success due to their low catalytic rates, we decided to focus on ribozymes with self-cleavage or ligation activities for further experiments. Postdoc Dennis Mishler has concentrated on studying how RNA structure, misfolding, and thus the catalytic rates and efficiencies of various sequences are affected by different environmental conditions, principally temperature. New kinetic simulations predicted that the RNA sequences most likely to benefit from conditions that cause fold sampling are those that have a) high chances of misfolding and b) high catalytic rates. Using the HDV ribozyme, we experimentally validated these models for a small number of RNA sequences predicted to misfold, achieving modest increases (~3 fold) in product relative to controls when they were incubated at higher temperatures. We then created a library of >10,000 HDV ribozyme sequences with additional random sequences, which may cause misfolding, appended outside of the enzyme core. We are in the process of analyzing the activities of these sequences at different temperatures using Illumina deep sequencing data as a high-throughput way of quantifying the advantages of fold sampling. (2) Dr. Mishler also began a computational and experimental project to study RNA fitness landscapes around two unrelated ribozymes with overlapping neutral networks previously studied by the Bartel lab. This project will determine whether fold-sampling results in a greater number of neutral mutational pathways in sequence space between these two distinct ribozyme folds by using RNA folding algorithms and a similar next-generation sequencing approach.

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

Peroxisomes are organelles that sequester various oxidative reactions, thereby protecting cytosolic constituents from oxidative damage. Peroxisomes are essential in plants and humans, but small molecules that specifically modulate peroxisome biogenesis, protein import, or maintenance are lacking. We have developed positive screens for both decreased peroxisome function in wild type and increased peroxisome function in peroxisome-defective mutants. We are exploiting these screens to identify compounds that inhibit peroxisome functions in wild type or enhance peroxisome functions in mutant backgrounds.

We are screening chemical libraries from the John. S. Dunn Gulf Coast Consortium for Chemical Genomics. We use the smaller Microsource Spectrum Collection (2,000 compounds: 1,040 drugs, 800 natural products and derivatives, and 160 toxic substances) in pilot studies and the larger Maybridge HitFinder Collection (14,400 compounds selected for structural diversity) for scale-up. We have identified three peroxisome inhibitors and several compounds that appear to restore peroxisome function to a mutant. We currently are conducting structure-activity assays on our lead compounds, exploring candidate target proteins, and continuing to screen the Maybridge collection. We expect to uncover new molecular tools with which to elucidate and modulate the biogenesis and function of these essential organelles.

MIKHAIL A. BELKIN, F-1705, The University of Texas at Austin. PLASMONIC-ENHANCED NANOSCALE MID-INFRARED MICROSCOPY WITH MONOLAYER SENSITIVITY.

We have attained all year two goals. Nanospectroscopy with monolayer sensitivity based on detecting molecular photoexpansion forces was demonstrated using samples made of monolayer islands of poly(ethylene glycol) methyl ether thiol and 4-nitrothiophenol molecules. Sub-monolayer sensitivity and better than 25 nm resolution was achieved in ambient conditions. These results were presented as an invited talk at SciX conference in Milwaukee, WI in October 2013 and in the paper published in *Nature Photonics* in April 2014

We have also developed and experimentally demonstrated an approach to suppress the parasitic signal due to substrate and atomic force microscope (AFM) tip expansions using a second laser source. The method is based on discriminating between sharp absorption peaks of the samples and broadband featureless absorption of the metalized substrate and the AFM tip. The results were reported at CLEO conference in June 2014; further presentations of this method are planned at the 2014 SciX and 2015 Pitcon conferences. Finally, we have developed a technique and obtained initial proof-of-concept results for mid-infrared photoexpansion nanospectroscopy in aqueous environments with ~100 nm spatial resolution.

The PI, Dr. Mikhail Belkin, was selected to be the 2014 Society for Applied Spectroscopy Tour Speaker based on the results of this project. The findings of this project are now being transferred into commercial nanoscale infrared microscopy instrument (NanoIR-2) produced and marketed by Anasys Instruments (www.anasysinstruments.com) with the support of the U.S. Department of Energy Phase 11 STTR award.

NICOLE A. BENEDEK, F-1803, The University of Texas at Austin. UNDERSTANDING THE CRYSTAL CHEMISTRY OF BI-BASED PEROVSKITES.

In the first year of the project we investigated the structures and possible ferroelectric properties of a series of Dion-Jacobson phases. Specifically, we were interested in understanding the driving force for the formation of a ferroelectric structure in CsBiNb₂O₇ and CsNdNb₂O₇, considering the former compound contains a stereochemically active lone pair cation (Bi³⁺), whereas the latter compound does not. We found that a novel form of ferroelectricity we identified in previous work (termed hybrid improper ferroelectricity) could provide a unifying explanation for the emergence of polar structures in the Dion-Jacobson family. This mechanism is driven by a combination of two non-polar lattice distortions (so-called 'rotations' of the NbO₆ octahedra), which together establish the polar/ferroelectric lowest energy structure. This mechanism is also the driving force for ferroelectricity in CsBiNbO₇, despite the stereochemically active Bi cation. We also predicted that CsLaNb₂O₇, a material that so far has only been characterized as non-polar, should also adopt a polar structure below room temperature. Our experimentalist colleagues have synthesized the material and preliminary experimental work appears to confirm our prediction that the material is indeed polar below room temperature. This work was published in the *Journal Inorganic Chemistry*. I was also invited to present the work at the Workshop on the Fundamental Physics of Ferroelectrics and Related Materials in Washington, DC in January 2014. I gave a contributed talk at the March Meeting of the American Physical Society in Denver in March 2014 and will be presenting the work as a poster at the Gordon Research Conference on Solid-State Chemistry in July 2014.

MATTHEW R. BENNETT, C-1729, Rice University. DYNAMICAL CONSEQUENCES OF PROTEIN CHEMISTRY IN SYNTHETIC GENE CIRCUITS.

In the past year we have analyzed the effect of mutations to LacI on the dynamics of synthetic gene circuits. For instance, we examined how chimeric proteins containing the DNA-binding domain of LacI and the ligand-binding domain of other transcription factors from the same protein family can co-regulate gene transcription from the Lac promoter. By altering the ligand-binding domain of LacI, we are able to change the ligand specificity of the transcription factor. We showed that up to four different chimeras, each of which responds to a different ligand, could be used simultaneously to regulate a single promoter. This work is currently submitted to *ACS Synthetic Biology*.

We have also published numerous articles over the past year. These include one in which we found thermo-stability of transcription factors can alter the dynamics of gene circuits. Specifically, we were able to create a synthetic gene oscillator that exhibits temperature compensation – an enigmatic feature of circadian oscillators. That study was published in *Proc. Natl. Acad. Sci. USA*. We are now working on understanding the fundamental chemistry behind this important mutation. We want to know what characteristics it confers to the protein. In other studies, we have begun examining how enzymatic processing of transcripts affects the signaling times of transcriptional cascades. We are beginning to experimentally test some of our theories by mutating transcription factors to alter their signaling dynamics.

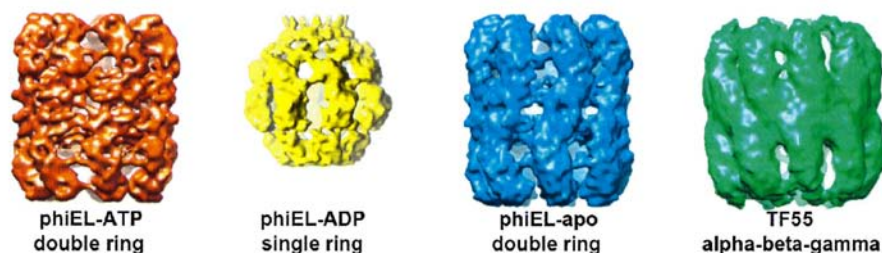
DAVID E. BERGBREITER, A-0639, Texas A&M University. THERMALLY RESPONSIVE MULTIPHASIC CATALYST SYSTEMS.

In the past year, our Welch support led to three published papers. One other paper has been accepted for publication but has not appeared in print in the journal. These papers described several topics. One was an invited perspective that described the state of the art for soluble polymers as tools in catalysis, discussing the future of this expanding area. A second paper discussed the ways I use examples of our Welch Foundation supported research in my award-winning undergraduate teaching providing examples that other could use in their sophomore organic chemistry classes. A third paper described our ability to use polyisobutylene (PIB) to make otherwise insoluble metallophthalocyanines soluble. The results of this study showed that metallophthalocyanines with FIB substituents are soluble at concentrations up to 20 weight percent in nonpolar or modestly polar solvents – a result that makes these compounds potentially useful as homogeneous catalysts for a range of transition metal catalyzed processes. Another paper was accepted for publication and is published on the web. This described new roles for soluble phase selectively soluble polymers in catalysis. Using a PIB-bound Rh(II) carboxylate catalyst in a heptane/acetonitrile mixture we showed that we could use the phase selective solubility of this catalyst to suppress bimolecular side reactions of the acetonitrile soluble ethyl diazoacetate reactant used in cyclopropanation and O-H insertion reactions. This paper further showed that inexpensive unfunctionalized soluble polymers can also serve as antileaching agents – a completely new role of soluble polymers in catalysis. Finally a fifth paper describing synthetic routes to highly heptane phase selectively soluble polystyrene derivatives was accepted but is not yet in print or on the web.

RICARDO A. BERNAL, AH-1649, The University of Texas at El Paso. ELUCIDATION OF A NOVEL MECHANISM USED BY A VIRUS ENCODED CHAPERONIN.

The research project has seen significant progress since we began data collection on our new cryo-Electron Microscope. We are getting closer to determining the complete protein folding pathway for the phi-EL chaperonin using cryo-electron microscopy. We have submitted the manuscript to *PLoS One* but reviewers requested that we run analytical centrifugation to prove the existence of the single ring protein folding intermediate. Since we do not have analytical centrifugation capabilities on our campus, we have sent our samples to be analyzed at UT Health Science Center San Antonio and are awaiting results. We have also started a project to study TF55, a chaperonin from *Sulfolobus solfataricus*. This chaperonin is composed of three proteins (α - β - γ) that are arranged into a 9 subunit ring with three-fold dihedral symmetry (green in figure below). At this point, the TF55 chaperonin needs further refinement and it is anticipated that we will publish this structure at the end of this year. We have also started collecting data on the human mitochondrial chaperonin hsp60/10. We have collected data on this chaperonin and have only a preliminary reconstruction at about 15 angstrom resolution. This reconstruction has been

particularly challenging because the chaperonin is in many different conformations. We are computationally separating the conformational states and will generate a reconstruction for each one. This should give us a good idea of the different conformations that it goes through in its normal protein folding pathway.



JOHN W. BEVAN, A-0747, Texas A&M University. STRUCTURE AND DYNAMICS OF PROTOTYPICAL HYDROGEN BONDED AND RELATED INTERACTIONS.

Supersonic jet and other spectroscopic methods have been developed and used to generate precise experimental data for morphing potentials and revealing fundamentally new characteristics in isolated prototypical hydrogen bonded and related interactions. The operation of the recently developed quantum cascade laser (QCL) supersonic slit jet spectrometer now has a $\times 100$ upgraded in sensitivity for pulsed operation permitting characterization of hetero-molecular interactions of H_2O such as H_2O-CO , H_2O-N_2 and open shell complexes. In addition, different classes of ground electronic state pairwise interatomic interactions have also been referenced to a single canonical potential using explicit transformations. These approaches have been applied to diatomic molecules N_2 , CO , H_2^+ , H_2 , HF , LiH , Li_2 , CO , O_2 ; argon dimer, and one-dimensional cuts through multidimensional potentials of $OC-HBr$, $OC-HF$, $OC-HCCH$, $OC-HCN$, $OC-HCl$, $OC-HI$, $OC-BrCl$, and $OC-Cl_2$ using accurate semi-empirically determined interatomic Rydberg-Klein-Rees (RKR) and morphed intermolecular potentials. The different bonding categories represented in these systems vary from van der Waals, halogen bonding, hydrogen bonding to strongly bound covalent molecules with binding energies covering three orders of magnitude from 84.5 cm^{-1} to 89600.6 cm^{-1} in ground state dissociation energies. Such formulations were then utilized to give a unified perspective on the nature of bonding for the whole range of diatomic and intermolecular interactions investigated.

ILYA B. BEZPROZVANNY, I-1754, Rice University. NOVEL AMYLOID-BINDING PEPTOID LIGANDS AS ALZHEIMER'S THERAPEUTIC.

Using on-beads peptoid screening technology we identified a specific Abeta42-binding peptoid IAM1. Using in vitro binding assay and Abeta aggregation assay we demonstrated that IAM1 interacts with Abeta42 with 20-fold higher affinity than with Abeta40. We reported identification and initial characterization of IAM1 in the last year publication (Lou at a (2013) *ACS Chem. Neurosci.*, vol 4, pp 952-962). Since publication of IAM1 discovery we have been focused on developing a system for evaluation of association between IAM1 and Abeta42 by crystallographic methods. We have been able to achieve some progress, but have not yet obtained diffraction quality crystals of IAM1 complexed with Abeta42. We will continue to develop this approach further.

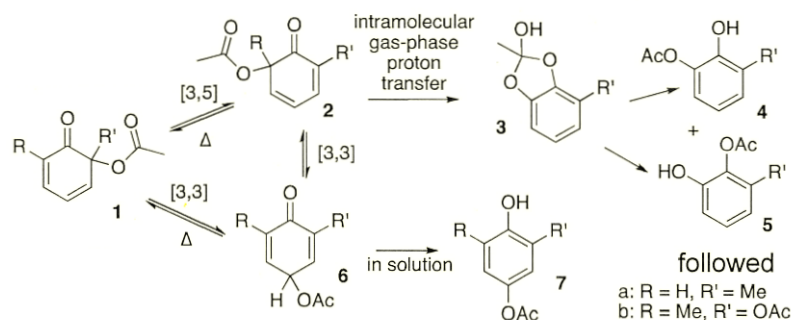
W. E. BILLUPS, C-0490, Rice University. CHEMISTRY OF CARBON NANOMATERIALS.

Electron irradiation of anthracite functionalized by dodecyl groups leads to recrystallization of the carbon network into diamonds. The diamonds range in size from $\sim 2 \text{ nm}$ to $\sim 10 \text{ nm}$ and exhibit $\{111\}$ spacing of 2.1 \AA . A bulk process consistent with bias enhanced nucleation is proposed in which the dodecyl group provides hydrogen atoms during electron irradiation. Recrystallization into diamond occurs in the hydrogenated graphitic subsurface layers. Unfunctionalized anthracite could not be converted into diamond during electron irradiation. The dependence of the phase transition pressure on cluster size was estimated, and it was found that diamond particles with a radius up to 20 nm could be formed.

Reduction of activated carbon using sodium in liquid ammonia results in a sodium/activated carbon salt that can be reacted with 5-bromovaleric acid to form water-soluble alkylcarboxylated activated carbon. The Zeta potential of this material was determined to be -32 mV , indicating a strongly negatively charged surface that contributes to the stability of the water suspension. A TEM image of a functionalized sample showed quasi-spherical aggregated particles with a size of $50-100 \text{ nm}$. The antibacterial property of the silver salt of the carboxylated activated carbon was evaluated by determining the MIC against a gram negative bacteria *E. coli* and found to be 38 \mu g/ml .

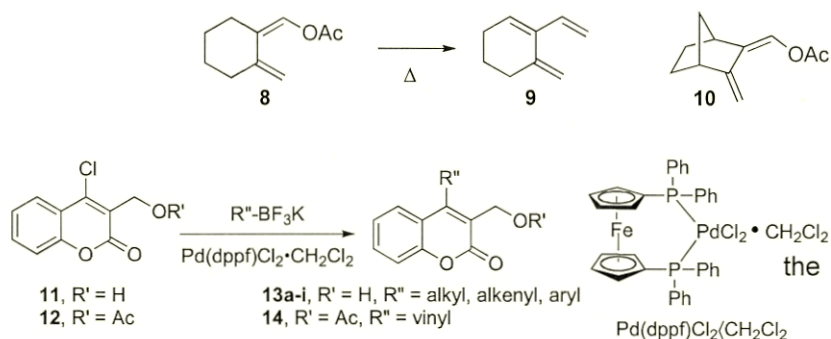
DAVID M. BIRNEY, D-1239, Texas Tech University. STUDIES OF PSEUDOPERICYCLIC AND PERICYCLIC REACTIONS.

(I) An experimental reinvestigation of the thermal rearrangements of 1a has shown that the major products are 4a and 5a, not 7a. Unexpectedly, raising the pyrolysis temperature increases the selectivity. This is explained by a mechanism calculated to involve favored pseudopericyclic [3,5]-sigmatropic rearrangement to 2a, by an unusual pseudopericyclic proton transfer to 3a, avoiding equilibration with 6a. Facile ring opening gives 4a and 5a, possibly a general mechanism for acyl migration. The intermediate 2b can be isolated. X-ray crystallographic studies support the argument that the [3,5] is pseudopericyclic.



(II) Several other 2,4-pentadieneol derivatives have been synthesized; studies of rearrangements of isoelectronic derivatives are underway. Attempts to observe rearrangements of 8 give only the elimination product 9. Synthesis of 10 is underway, which cannot eliminate, but only rearrange.

(III) Vinyl acetate 14 was also anticipated to possibly undergo 3,5-rearrangements. In seeking a synthetic route towards this compound, Pd(dppf) catalyzed couplings of II and 12 to form 13 and 14 were developed.



SIBANI L. BISWAL, C-1755, Rice University. CONTROLLING NANOPARTICLE ASSEMBLY VIA STERIC FORCES.

Controlling the assembly of nanoparticles into well-defined functional systems remains a challenge. The main difficulty is that the majority of bulk nanoparticle processing methods result in nanoparticle aggregation and phase separation. Top-down methods, for example, lithography, are popular and easy to perform but they are limited to the larger scale end and lack of the fine-tuning ability. This grant year, we developed a soft-templating strategy to direct the assembly of nanoparticles into higher ordered network structures. In the process, we discovered a novel method to create micron-sized rings from conjugated polymer nanoparticles using a mixed solvent evaporation method.

We also adapted a microcantilevers system for the characterization of lipid membrane and its interaction with nanoparticles. Supported lipid bilayers (SLBs) have served as a useful model for complex cell membranes. The main structural feature of SLBs is the asymmetry in the membrane environment: one membrane leaflet is exposed to an aqueous solution while the other is exposed to a solid support. We report how block copolymer nanoparticles crowd onto these membrane interfaces as a function of temperature. A Langmuir isotherm model and a free mean area theory were developed to explore the association of the copolymers with the SLBs and hindered lipid diffusion.

ERIC R. BITTNER, E-1337, University of Houston. THEORY AND SIMULATIONS OF ELECTRONIC DYNAMICS IN ORGANIC SOLAR CELLS

The dynamics of electron transfer and charge separation in polymer-based photovoltaic systems is dictated by a sequence of elementary steps following photo-excitation. First an exciton created within the bulk of the material must diffuse to a region of the material where there is an electronic driving force for charge-separation. Typically, this is at a phase boundary between a donor material and an acceptor material. Charge transfer states formed at the interface are typically Coulomb-bound electron/hole pairs (exciplex states) pinned to the interface leading to a decrease in both the photocurrent and power conversion efficiency. One of the fundamental questions in the field of polymer photovoltaics is how higher photocurrents can be achieved given that immobile states are thermodynamically favored.

In collaboration with Carlos Silva as a Fulbright Canada Scholar, we developed a model and performed a series of experiments that indicate that photocurrent can be produced directly and coherently from the excitonic states via dynamical tunneling. This article was reported in *Nature Communications* earlier this year. Our model suggests that rather than forming the thermalized state, excitons in fullerene/polymer blends dissociate *directly* to form current producing states.

More recently, we developed a new model for accurately computing energy and electron transfer rates taking input directly from quantum chemistry calculations. Our methods use localized states to define the initial donor and acceptor diabatic states. By computing analytical gradients of both ground and excited states (not an easy task!) we obtain the necessary coupling terms for computing golden-rule transition rates using a time-convolution less master equation approach. This work was just accepted for publication in *J Phys. Chem.*

PAUL BLOUNT, I-1420, The University of Texas Southwestern Medical Center. DETERMINING LIPID PROTEIN INTERACTIONS FOR A CHANNEL GATED BY MEMBRANE TENSION.

The MscL and MscS bacterial mechanosensitive channels directly sense and respond to membrane tension. We are in the process of designing experiments that allow us to determine the dynamics of these sensors within the membrane bilayer. We have made advances in determining the influence of specific lipids and protein-lipid interactions on the gating of both MscL and MscS.

The *M. tuberculosis* MscL channel was found 14 years ago to be non-functional when expressed in *E. coli*. In our last report we had submitted a paper demonstrating that inclusion of phosphatidylinositol, a lipid headgroup found in *M. tuberculosis* but not *E. coli*, is required for the normal gating of the *M. tuberculosis* MscL channel. This is now published. We have also found a region where protein-lipid electrostatics can define properties of MscL gating; this has been submitted.

For MscS mechanosensitive channel gating, we have submitted a paper on an apparent lack of specific residue-lipid interactions in the fatty acid region of the bilayer. On the other hand, we have generated numerous channels with single cysteine mutations at the lipid interface that have been screened with sulfhydryl reagents. In addition, we have generated and screened by patch clamp mutations at ten independent sites within the lipid interface regions. The preliminary studies from this work have been promising, and we are now focusing on one region from residues 114 to 127, which appears to play a large role in determining channel kinetics and the propensity of attaining an inactive state.

JANET BLUEMEL, A-1706, Texas A&M University. THE SONOGASHIRA CATALYST SYSTEM FOR C-C COUPLING REACTIONS: NEW MECHANISTIC INSIGHTS AND IMPROVED RECYCLABILITY.

Many basic questions about immobilized catalysts, and in particular the Sonogashira system, could be answered. **(a) Nanoparticles and catalysis:** Immobilizing a Rh hydrogenation catalyst on a nanoplatelet support leads to a recyclable catalyst with record activity. However, irregularly shaped Rh nanoparticles form at the onset of the catalytic reaction and their unlimited growth shortens the catalyst lifetime. It can be concluded that nanoparticle formation is independent of the support material and that they keep their size and shape only when confined in the pores of silica. **(b) Mobility studies:** Mono-, bi-, and tridentate phosphine ligands, covalently bound to the surface, have been offered to PdCl₂ during *in situ* competition experiments. Hereby, the migration of the Pd complex to one of two different linkers on the support has been monitored over time by ³¹P HRMAS. The coordinating strengths of the ligands have been ranked, and a correlation with the catalytic activity of the immobilized Sonogashira catalyst system has been established. Ligands that bind the Pd complex too strongly prevent the formation of Pd/Cu (1:1) nanoparticles on the support surface and thus lead to lower activity of the Sonogashira catalyst. **(c) Surface Adsorption:** The structures and dynamic processes of phosphine oxides and metal complexes, adsorbed on silica surfaces, have been investigated, and a method for visualizing the mobilities macroscopically has been developed.

JENNIFER S. BRODBELT, F-1155, The University of Texas at Austin. FUNDAMENTALS OF PHOTO- AND ELECTRON-BASED ACTIVATION OF IONS IN THE GAS PHASE.

Infrared multiphoton dissociation was used to investigate the distributions of intrastrand crosslinks formed between cisplatin and two oligodeoxynucleotides (ODN), d(A₁T₂G₃G₄G₅T₆A₇C₈C₉C₁₀A₁₁T₁₂) and d(A₁T₂G₃G₄G₅T₆T₇C₈C₉C₁₀A₁₁T₁₂), which adopt different secondary structures in solution. Two isobaric crosslink products were differentiated for each ODN. Comparison of the fragmentation patterns of the platinated crosslinks indicated that backbone cleavage was significantly suppressed near the crosslink. Ultraviolet photodissociation and a chemical probe strategy were used for the structural characterization of proteins to evaluate conformational changes as a function of denaturation. This strategy was applied to the third zinc-finger binding domain, domain C, of PARP-1 (PARP-C), to evaluate the discrepancies between the NMR and crystal structures which reported monomer and dimer forms of the protein, respectively. The trends reflected from the reactivity of each lysine as a function of acetonitrile denaturation in the present study support that PARP-C exists as a monomer in solution with a close-packed C-terminal alpha helix. Those lysines for which reactivity increased under denaturing conditions were found to engage in tertiary polar contacts such as salt bridging and hydrogen bonding. We developed negative mode ultraviolet photodissociation for the characterization of acidic O-linked glycopeptide anions, a method that afforded 100% sequence coverage of the peptide and glycan moieties. The most abundant and frequent peptide sequence ions were a/x-type products, which, importantly, were found to retain the labile glycan modifications. We designed an automated database searching strategy (based on the MassMatrix algorithm) that is specific for the analysis of glycopeptide anions by UVPD.

KATHLYNN C. BROWN, I-1622, The University of Texas Southwestern Medical Center. DESIGN AND SYNTHESIS OF TUMOR TARGETED DRUG DELIVERY SYSTEMS FOR LUNG CANCER THERAPY.

We finished characterization of the endocytic uptake of the $\alpha\beta6$ Integrin binding peptide, H2009.1. H2009.1 Is Internalized by a caveolar mechanism and does not localize in low pH endosomal or lysosomal compartments. Instead, 85% of the peptide accumulates within multivesicular bodies concentrated in the perinuclear region. $\alpha\beta6$ is internalized with the ligand but recycles back to the cell surface. Based on these data, conjugation of H2009.1

to drug molecules that can escape from neutral vesicles should be more effective than acid labile or protease-sensitive. Indeed, H2009.1 peptide conjugated to doxorubicin via a hydrazone linker is weakly cytotoxic. Yet, conjugation of biotinylated H2009.1 to streptavidin-saporin was highly cytotoxic to $\alpha\text{v}\beta\text{6}$ -positive cells but not cells that lack $\alpha\text{v}\beta\text{6}$.

To isolate peptides that traffic to acidic cellular compartments, we developed a phage display scheme that allows for selection of peptides that internalize into cells via known mechanisms of endocytosis. We identified a peptide LQWRDDNVHNFGVWARYRL (H1299.3) that utilizes clathrin-mediated endocytosis and co-localizes with Lamp1. We synthesized a nanoparticle system which displays H1299.3, on its exterior surface and encapsulates H250, an immunogenic HLA class 1 restricted peptide. This synthetic delivery system facilitates presentation of the immunogenic H250 peptide in MHC and HLA class 1 molecules as measured by CD8⁺ specific IFN γ secretion. Presentation is dependent on the targeting peptide and utilizes an autophagy-mediated mechanism to facilitate presentation. Treatment with this liposome results in a significant reduction in LLC1 tumor growth in vaccinated mice.

RICHARD K. BRUICK, I-1568, The University of Texas Southwestern Medical Center. ANALYTICAL APPROACHES TO CHARACTERIZE IRON- AND OXYGEN-SENSING MECHANISMS GOVERNING CELLULAR IRON HOMEOSTASIS.

FBXL5 is an iron- and oxygen-responsive subunit of an E3 ubiquitin ligase that governs the stability of Iron Regulatory Protein 2 (IRP2), an important posttranscriptional regulator of several iron metabolism genes. We've previously shown that FBXL5's N-terminus folds into a hemerythrin-like (Hr) domain that acts as an iron-sensitive conformational switch governing FBXL5's function. While we have learned a great deal regarding the roles of FBXL5 and its Hr domain in iron and O₂ sensing, many questions remain. The primary objectives of this proposal are to use sophisticated analytical techniques to (a) identify additional SCF^{FBXL5} substrates and to (b) characterize additional mechanisms by which FBXL5 is regulated by iron. We have completed an initial stable isotope labeling by amino acids in cell culture (SILAC) experiment to identify proteins differentially ubiquitinated as a function of cellular iron or as a function of FBXL5 availability. We prioritized these "hits" and are currently validating several leading candidates. Also, while the Hr domain plays a major role in mediating iron- and oxygen-dependent responses in the mammalian cellular iron homeostasis pathway, preliminary data suggests that there are additional mechanisms by which FBXL5 responds to these metabolic cues. For example, the ability of FBXL5 to recognize its IRP2 substrate is also iron-dependent. We have initiated work with the UTSW Mass Spectrometry Core Facility to search for candidate post-translational modifications that govern substrate recognition in an iron responsive manner. To complement these studies, we are engineering yeast to express FBXL5 with the goal of creating an orthogonal system to reconstitute iron regulation through complementation strategies.

KEVIN BURGESS, A-1121, Texas A&M University. HYDROGENATIONS OF STEREOCHEMICALLY COMPLEX SUBSTRATES: THE END OF A MESSY DIVORCE AND THE BEGINNING OF A NEW ROMANCE.

In this grant period we completed and published our work on syntheses of ligands via metathesis to generate catalysts *in situ*. In retrospect we realize that the building blocks used were sub-optimal for catalyst design, but proof of principle was obtained (Figure 1).

We also completed and published work on combining organocatalysis with asymmetric hydrogenations to develop a synthesis of homo-Roche ester derivatives (Figure 2). This work provides an efficient, and scalable route to useful synthons that have not been applied as widely as might be expected, probably due to accessibility.

Our other work in this area featured a side-by-side comparison of chiral Crabtree's catalyst analogs with carbene ligands having different degrees of unsaturation.

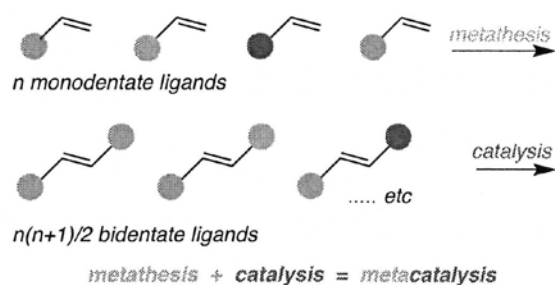


Figure 1. Metathesis to form ligands *in situ*.

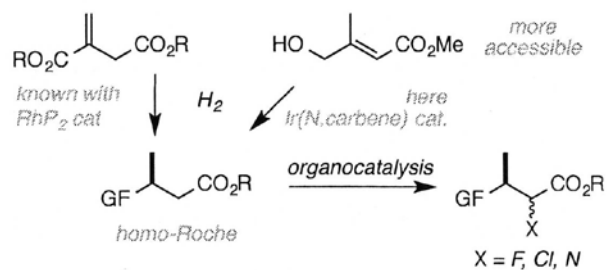


Figure 2. Serial asymmetric hydrogenation and organocatalysis.

SHAWN C. BURGESS, I-1804, The University of Texas Southwestern Medical Center. DYSREGULATION OF INTRACELLULAR LIPID SYNTHESIS DURING DISEASE.

Intracellular lipids and their synthesis contribute to the mechanisms and complications of obesity associated diseases. We described an NMR approach that provides an abbreviated lipidomic analysis and concurrent lipid biosynthetic fluxes. Following deuterated water administration, positional isotopomer analysis of specific lipid species by deuterium NMR reported flux through de novo lipogenesis (DNL), fatty acid (FA) elongation, desaturation and triglyceride-glycerol synthesis. The NMR method obviated certain assumptions regarding sites of enrichment and exchangeable hydrogens required by mass

isotope methods. The method was responsive to genetic and pharmacologic gain or loss of function of DNL, elongation, desaturation and glyceride synthesis. Obese and insulin resistant BDF1 mice consuming a HFD for 35 weeks were examined across feeding periods to determine flux through these pathways during insulin resistance and high fat consumption. High fat feeding resulted in increased rates of fatty acid elongation and glyceride synthesis but, DNL was massively suppressed despite insulin resistance and obesity. We concluded that high fat consumption by mice suppresses lipogenesis even during obesity and insulin resistance.

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

Molecular level design of functional soft materials through the self-assembly of microscopic building blocks (molecules, colloids, etc.) will be a major focus of research for the foreseeable future. To sort through the large parameter space of molecular architecture, advance molecular theories need to be employed to understand how molecular interactions control nanoscale or mesoscale structuring and therefore macroscopic properties. The molecular density functional theory (DFT) developed in this research is filling this need - offering distinct advantages in considering trace components, explicit solvent, and short-ranged, directional association sites. Sandia National Lab continues to adopt advances in the theory in their open source Tramoto package, enabling wide use of the theory in academia, national labs, and industry.

In the past year, research has focused on two of the microscopic building blocks with wide impact: patchy colloids and surfactants. To enable interpretation of new experiments on patchy colloids, we extended the theory for patchy colloids to allow for spherically symmetric association sites and bond angle dependence resulting in steric hindrance, ring formation, and double bonding. We also extended the theory to allow for cooperative association (non-pairwise additive interactions) that is of key significance for associating molecules. We have demonstrated molecular level explanation of experiments involving water in a hydrophobic solvent, grafted copolymer brush surfaces that transition from hydrophilic to hydrophobic with temperature, and the surface activity of alcohols. Further development of the theory will focus on interfacial properties of patchy colloids as well as surfactants.

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 twenty-two papers in *Nature Commun.*, *J. Am. Chem. Soc.*, *Energy Environ. Sci.*, *Chem. Commun.* and *J. Mater. Chem. A* etc together with three accepted articles and one submitted manuscript. The most important progress is the realization of a unique microporous metal-organic framework with the record methane working capacity (*J. Am. Chem. Soc.*, 2014, 136, 6207) and establishment of an empirical formula to predict methane storage capacities (*Energy Environ. Sci.*, 2013, 6, 2735). We, for the first time, discovered the application of metal-organic framework for lasing application (*Nature Commun.* 2013, 4, 2719 (DOI: 10.1038/ncomms3719)). Furthermore, we significantly enhanced the sensitivity of the metal-organic framework thermometers based on mixed-lanthanide metal-organic framework materials (*J. Am. Chem. Soc.* 2013, 135, 15559). Because of our leading status in this very active research field, we have been invited to write a series of review and perspective articles which have been published and accepted in *Coordination Chemistry Reviews* (2014, 273-274, 76), *Chemical Society Reviews* (two online published reviews: 2014, DOI: 10.1039/C4CS00032C and DOI: 10.1039/C4CS00041B), and *Energy Environ. Sci.*, (2014, DOI: 10.1039/C4EE00143E). My significant achievement in chemistry research has been recently recognized by Thomson Reuters in which I have been selected as one of the Highly Cited Researchers 2014 in Chemistry (<http://highlycited.com>) and THE WORLD'S MOST INFLUENTIAL SCIENTIFIC MINDS 2014 (<http://sciencewatch.com/grr;presenting-highly-cited-researchers>). It is my great pleasure and honor to share such a prestigious recognition with those leading scientists such as Robert H Grubbs from California Institute of Technology and George M Whitesides from Harvard University. I would like to take this opportunity to thank Welch Foundation for the generous and continuous support for my ongoing research which has made such recognition possible for me.

CHUO CHEN, I-1596, The University of Texas Southwestern Medical Center. MECHANISTIC STUDIES ON THE VANADIUM-CATALYZED C-H HYDROXYLATION REACTIONS.

In the previous grant period, we successfully completed the initial goal of understanding how vanadium complexes catalyze the oxidation of hydrocarbons. We have thus extended our efforts to developing other C-H oxidation reactions. We have successfully identified an efficient vanadium catalyst system for promoting C-H fluorination reactions. We have also discovered a photochemical process for catalyzing C-H fluorination reactions using cheap, readily available organic ketones. Selective mono- and difluorination at benzylic positions as well as selective fluorination of unactivated positions could be achieved by catalyst control. Taken together, the Welch research funds have fueled the development of several chemical transformations that are particularly useful in medicinal chemistry and material sciences.

During this grant period, we have also found that visible light can promote photoreactions of simple unsaturated ketones despite no significant absorption. Visible light is a cheap, sustainable, and readily available source of energy input for chemical reactions. While plants and bacteria are well-known for their ability to harvest visible light to promote redox reactions, synthetic chemists mostly use UV light to promote photoreactions. This is because simple organic molecules usually do not absorb visible light. We believe that visible light has broader utilities than generally anticipated. We are currently exploring the potential use of visible light to promote a series of new and classic photoreactions.

ZHENG CHEN, AU-1731, The University of Texas Health Science Center at Houston. MOLECULAR MECHANISMS OF ACTION OF CLOCK-MODULATING SMALL MOLECULES.

The first study aims to identify protein targets of Nobiletin/CEM5, a clock-enhancing polymethoxylated flavonoid showing robust clock-dependent metabolic efficacy (He et al., in revision). Using cell-based reporter assay, we first ruled out a role of Nobiletin (NOB) as a direct ligand for PPAR γ , a key nuclear hormone receptor identified as a downstream effector of NOB. In a major breakthrough, collaborative work with Dr. Young-Ger Suh led to identification of a biotinylated NOB derivative retaining ~45% of its clock-enhancing activity. Using this excellent reagent, we methodically optimized conditions for biochemical pull-down using whole and fractionated cell extracts. Among the potential bands of interest, one band at ~61KD has been reproducibly observed in four separate pull-down experiments. With further enrichment, mass-Spec protein ID is being conducted by Dr. Jun Qin's lab at BCM across the street. In another study, we have identified the transcription factors C/EBPs (both α and β) as key cellular targets of NOB. We showed that enhanced expression of C/EBPs activates circadian transcription of their target gene *Cps1*, which encode the rate-limiting enzyme of the urea cycle, carbamoyl phosphate synthase I. As a result, CPS1 proteins accumulate in mouse liver following NOB treatment, and importantly, function to maintain homeostasis of serum ammonium levels. This study reveals a NOB-dependent mechanism of action important for amino acid metabolism, and elucidates pivotal transcription factors as cellular mediators of this small molecule (Nohara et al., in preparation). Finally, extending previous observations in cell culture, we are characterizing the mouse tissue clock function of CEM3, a clock-enhancing benzimidazole with the unique ability to enhance the master pacemaker in the hypothalamic suprachiasmatic nuclei.

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

Mitochondrial Anti-Viral Signaling (MAVS) protein is essential for the induction of type-I interferons and other cytokines in response to infection by RNA viruses such as Influenza. We have previously shown that virus infection leads to a massive aggregation of MAVS on the mitochondrial outer membrane and that MAVS aggregation is required for the activation of cytosolic kinases IKK and TBK1, which activate the transcription factors NF- κ B and IRF3, respectively. NF- κ B and IRF3 then enter the nucleus to turn on type-I interferons. Remarkably, MAVS forms prion-like polymers which can convert endogenous MAVS into functional aggregates. Our recent studies showed that MAVS polymerization through the N-terminal CARD domain allows the intermediate domain, which contains several TRAF-binding sites, to recruit and activate TRAF proteins, including TRAF2, TRAF5 and TRAF6. These TRAF proteins then function as ubiquitin E3 ligases to activate IKK and TBK1. More recently, we employed the yeast prion assay to demonstrate that the MAVS CARD domain is indeed a bona fide prion. Further, in a screen to identify other mammalian prion-like domains, we found that the PYRIN domain of the inflammasome adaptor ASC is also a prion domain. Mutations that disrupt the prion filament formation of ASC abrogate its ability to activate the inflammasome complex. We also discovered an inflammasome-like pathway in fungi that is activated through the prion conversion mechanism. Thus, prion-like polymerization is an evolutionarily conserved mechanism of signal transduction that underlies a highly sensitive and robust response to infections and other noxious insults.

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 have measured the ability of human Brd4 binding to p300-acetylated HeLa chromatin, in the presence or absence of Hit-G and Hit-I small compound inhibitors that target a phosphorylated region of Brd4 named the N-terminal cluster of CK2 phosphorylation sites (NPS). We found that Brd4 binding to acetylated chromatin, determined by co-immunoprecipitation of acetylated chromatin with immobilized Brd4 protein and then monitored by Western blotting with anti-histone H3 antibody, is abolished by inclusion of Hit-G compound in the binding reaction. This inhibition is caused by disruption of intramolecular contact between NPS and a downstream basic residue-enriched interaction domain (BID), leading to "freed" NPS binding to the bromodomain and thus masking bromodomain-mediated Brd4 binding to acetylated chromatin. The Hit-G-inhibited Brd4 binding to acetylated chromatin is an activator-dependent process occurring in a gene-specific manner as evidenced by cell-based assays.

For Objective II, we found that addition of Hit-G compound in the cell culture medium significantly inhibits estrogen-induced estrogen receptor alpha (ER α) target gene transcription and also doxorubicin-induced p53 target gene transcription, as conducted by measuring RNA levels of a subset of ER- and p53-regulated genes by quantitative RT-PCR. Interestingly, only expression of select ER target genes, such as c-MYC, progesterone receptor, pS2 and CXCL12, but not GREB1, PKIB, SGK3 and RPL13A, as well as p53-targeted p21, but not HDM2, PUMA and TIGAR, is inhibited by Hit-G. These data suggest that: 1) Hit-G compound indeed inhibits Brd4-regulated gene transcription in an activator-dependent and gene-selective manner; and 2) Hit-G compound inhibits Brd4 binding to acetylated chromatin without blocking activator interaction with Brd4.

WAH CHIU, Q-1242, Baylor College of Medicine. STRUCTURAL STUDIES OF VIRUS BY Cryo-EM.

In the current grant period, we completed a structural study to use Zernike phase contrast (ZPC) electron cryo-tomography (CryoET) to follow the maturation process of wild-type cyanophage Syn5 as it occurs inside its host, *Synechococcus sp.* WH8109. Zernike phase contrast cryoET significantly enhance the low-frequency information, allowing for in-focus, high contrast imaging. Consequently, it facilitates the direct identification of many subcellular components, including thylakoid membranes, carboxysomes and polyribosomes, as well as newly synthesized phages, inside the congested cytosol of the infected cell. We reconstructed 58 ZPC tomograms of the cells. The computational classification of 470 sub-volumes of Syn5-like particles of similar shape and size resulted in five morphological types, which represent the syn5 particles in different maturation states. Most of these particles except the infectious

particles have never been biochemically purified. Our approach demonstrated the power of this new imaging modality to discover structures of possibly short-lived molecular machines undergoing a biological process like virus maturation in the host cell. In parallel, we also pursued the structural determination of biochemically purified syn5 phages using single particle cryo-electron microscopy. Our 4.7 Å resolution structure of syn5 phage showed the major capsid protein (gp39) to have a classic phage protein fold. Additionally, two knob-like proteins (gp55 and gp58) protruding from the capsid surface are observed with unexpected structural organization, which breaks all expected local symmetries and has never been observed in any known virus structures. Such non quasi-equivalence arrangement of the protruding proteins suggests a new mechanism in maintaining capsid stability in mature phage.

YUH MIN CHOOK, I-1532, The University of Texas Southwestern Medical Center. QUANTITATIVE CHARACTERIZATION OF NUCLEAR EXPORT INHIBITION.

Many CRM1 cargos are tumor suppressors, cell growth regulators or apoptotic factors that are misregulated and mislocalized to the cytoplasm in cancer cells. CRM1 is also overexpressed in several malignancies and elevated CRM1 is associated with lower survival rates in the patients. CRM1 inhibition restores nuclear localization and functions of tumor suppressors, leading to apoptosis of the cancer cells. Last year we reported an unexpected mechanism of inhibition of CRM1 by the older toxic natural product inhibitor Leptomycin B (LMB) and we found that the new KPT inhibitors (KPT-330 or Selinexor is currently in twelve phase one and two clinical trials for various cancers) developed by our collaborators at Karyopharm Therapeutics has a different mechanism of inhibition from LMB. Although KPTs bind covalently to CRM1, they are not irreversible inhibitors like LMB but are in fact slowly-reversible inhibitors. Slowly reversible CRM1-KPT interactions may contribute to their improved tolerance in animals since withdrawal of the drug may allow sufficient inhibitor release from CRM1 and allow essential nuclear export to resume in normal cells. In the past year, we have determined crystal structures of CRM1 bound to additional KPT compounds (common trifluoromethyl phenyl triazole scaffolds and variable Michael acceptor sidechains). The seven new structures show how inhibitors KPT-305, KPT-320, KPT-330/Selinexor, KPT-335/Nerdinexor (approved for treating canine lymphoma), KPT-348, KPT-350 and KPT-355 bind CRM1. We are performing large-scale comparative structural and biochemical analysis of the seven CRM1-KPTs, and will combine our results with Karyopharm's pharmacokinetics/pharmacodynamics and cytotoxicity results for a Structure Activity Relationship (SAR) type study.

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

Pyruvate dehydrogenase kinase isoforms (PDKs 1-4) negatively regulate activity of the mitochondrial gatekeeper the pyruvate dehydrogenase complex (PDC) by reversible phosphorylation. PDK isoforms are up-regulated in obesity, diabetes, heart failure and cancer and are potential therapeutic targets for these important human diseases. Recently, we employed structure-guided design to develop a series of highly specific PDK inhibitors that bind to the ATP-binding pocket. The final product of this series 2-[(2,4-dihydroxyphenyl)sulfonyl]isoindoline-4,6-diol is designated PS10. The administration of PS10 at 70 mg/kg to diet-induced obese mice significantly augments PDC activity in the liver, resulting in improved glucose tolerance with hepatic steatosis in this mouse model. These findings support the pharmacological approach of targeting PDKs to control both glucose and fat levels in obesity and type 2 diabetes.

In parallel, we performed the high-throughput screening of a small chemical library and identified a new class of inhibitors represented by 3,6-dichlorobenzo[b]thiophene-2-carboxylic acid (BT2), which are specific for the related mitochondrial branched-chain α -keto acid dehydrogenase kinase (BDK). BT2 exhibits good stability *in vivo*, and requires low doses for the long-term treatment. The discovery of benzothiophene carboxylate derivatives as stable BDK inhibitors provides the framework for a pharmacological approach to metabolic diseases caused by aberrant oxidation of branched-chain amino acids.

ABRAHAM CLEARFIELD, A-0673, Texas A&M University. METAL PHOSPHONATES AS CRYSTAL ENGINEERED SOLIDS AND PLATFORMS FOR DRUG DELIVERY.

During the past year progress was made in three areas of research listed above. α -ZrP particles were prepared with layered structures of about 50-150 nm and thicknesses of two to ten layers. The phosphate P-OH groups on the surfaces of the ZrP particles could be bonded to silanes, isocyanates, acrylates, phosphates, phosphonic acids and polyethylene glycols (PEGs). To bond phosphates and phosphonic acids to the surface, a layer of Zr^{4+} or Sn^{4+} ions are first placed on the surfaces by replacement of the surface protons. The phosphates and phosphonic acids then bond to the new metal ion surfaces. This broad range of surface functionalization procedures allows us to control the hydrophobic-hydrophilic character of the particles so that they can be dispersed in water, alcohols and a broad range of organic solvents. This has allowed us to prepare polymer composites, to bind Wilkinson's catalyst to the surface to carry out hydrogenation reactions, and also create a lubricant that shows promise of being an excellent metal polishing agent.

A one step hydrothermal synthesis of 1, 3, 5- benzene triphosphonic acid and NH_4^+ and $CH_3NH_3^+$ was used to prepare Zinc complexes that contained MOF type pores. These MOFs exhibited reversible dehydration as determined by *in situ* X-ray diffraction and NMR. Three different phases were obtained and their structures determined. The NH_4^+ could be replaced by Li^+ . An aluminum carboxymethyl-phosphonate was also prepared with NH_4^+ . The structure formed chains of six coordinate Al held together by hydrogen bonding to the ammonium ions.

Excellent progress has been made with our drug delivery program. As of this writing insulin, doxorubicin, cisplatin, titanocene and molybdocene have been intercalated between the layers of α -ZrP. Both the doxo and cisplatin materials have been administered to a number of breast cancer cells. The release of the drug has been followed by dyes fixed to the surface and confocal microscopy. High levels of cell destruction of the cancer cells were observed. Trials with synthetic blood have shown no release of the drugs outside the cancer cells. Several types of polyethylene glycols (PEGs) were bonded to the α -ZrP surfaces which did not displace the drugs. Trials with the particles covered with PEGs are in process. We are now also examining whether neurologically

active amine type drugs can be intercalated into the α -ZrP particles.

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

During this last year of funding, our research supported by the Welch Foundation has continued in two parallel lines: (1) We have been focusing on the study of the anomalous folding mechanism of the spectrin protein family. We have used our multiscale modeling and a procedure to incorporate experimental data into the modeling (previously developed by our group) to obtain the distribution of energy on the proteins. We have found significant differences among the three proteins that can explain their different folding behavior. We are collaborating with experimentalists to test our findings. One paper is in preparation. (2) We have combined ensemble sampling methods and the cloning/destroying ideas used in supersymmetric molecular dynamics with the knowledge of the slowest directions of motion along the dynamics that is obtained by our previously developed LSDMap approach. This allows "steering" the ensemble dynamics towards free energy barriers "on-the-fly" and significantly accelerating the sampling of rare events. Two publications resulted from this activity (one published, one in press). We have also applied this approach to several systems, most notably the characterization of the peptide IGDNINDFK used in a metalloprotein catalyst, in collaboration with an organic chemist. The combination of the coarse-graining approach with the fast exploration methodology at atomistic resolution will allow us to study at multiple resolutions the dynamics and thermodynamics of biomolecules that are completely out of reach with existing methodologies. We are currently studying the slow conformational dynamics of a glutamate receptor protein.

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

We have completed the structure of an ERK2 mutant associated with human cancers. The mutation disrupts the docking site on ERK2 for protein substrates. The mutant also dimerizes less well with wild type ERK2 and homodimerizes poorly. These findings again support the idea that there is communication between the ERK2 dimer interface and the substrate docking site. The C-terminal domain and activation loop are less ordered. The activation loop assumes a position similar to the activation loop in the active structure which may increase its activation in cells. This observation supports the conclusion that the docking site and the activation loop are energetically coupled.

We have also evaluated ERK2 activation loop plasticity by studying the effect of phosphorylation of T188 of ERK2 on its activity and DNA binding. This residue lies in the P+1 pocket which binds the residue immediately after the phosphorylation site in kinase substrates. This residue is highly conserved among the protein kinases and this threonine interacts with the catalytic base in some kinase crystal structures. This protein has low kinase activity but the pT188 form of ERK2 binds *in vitro* to oligonucleotides from several gene promoters better than unphosphorylated ERK2. Binding of ERK2 phosphorylated on the activating residues, Y185 and T183, is roughly equivalent. Crystallization experiments are ongoing.

For Aim 3, we are making WNK1 peptides to identify the smallest that binds the p85 cSH2 for structural analysis.

JEFFERY L. COFFER, P-1212, Texas Christian University. HOLLOW SEMICONDUCTOR NANOTUBES: STRUCTURAL AND COMPOSITIONAL CONTROL.

Work on this project within the past twelve months has centered on fundamental studies of the infiltration of selected magnetic nanoparticles into hollow silicon nanotubes (SiNTs), and an investigation of the effects of physical confinement of these nanoparticles in the nanotube interior as a function of nanotube wall thickness. Superparamagnetic Fe₃O₄ nanoparticles of different sizes (4, 5, 8 and 10 nm) were loaded into SiNTs with 10 and 70 nm wall thicknesses and a 50 nm inner diameter. Measurements of the blocking temperatures for such structures reveal interestingly low T_B values of 12K for the 4 nm Fe₃O₄ nanoparticles loaded into both the 10 nm as well as 70 nm thick SiNTs, indicating that the iron oxide particles are effectively shielded by tube walls and do not interact magnetically. Another remarkable result is the difference in T_B values in the case of SiNTs from that of porous silicon prepared from the anodization of crystalline Si with a comparable pore width (but different morphology). For Fe₃O₄ nanoparticles of 8 nm average diameter infiltrated into SiNTs, a T_B value of 20 K, equal to the T_B of isolated iron oxide particles of this size, is found. In contrast, the same particles filled into porous silicon offering an equivalent pore-diameter show a high value of T_B (~ 170 K), the latter readily explained by dipolar coupling between the particles within the pores. Complementary experiments concerning the influence of nanotube surface functionalization on related nanotube properties, using silicon alkoxide coupling chemistry, are currently under investigation.

DON M. COLTART, E-1806, University of Houston. NEW CATALYTIC ASYMMETRIC CARBON-CARBON BOND FORMING METHODS.

The focus of the grant proposal in question is the development of new catalytic asymmetric methods using aza- and nitrosoalkene substrates. To date, our research has focused on two primary objectives. The first of these is the asymmetric α -alkylation of chiral α -epoxy sulfonylhydrazones. We have found that the Cu(I) catalyzed addition of a certain Grignard reagents proceeds effectively in the case of six-membered ring systems and in a highly *anti*-selective manner to give β -hydroxy sulfonylhydrazones. Such products should be of considerable value in the synthesis of natural products, and investigations of their general utility in that regard are planned for the coming period of grant support. During the course of these studies we discovered a very interesting complimentary transformation, with regard to the stereochemical outcome. Further analysis and optimization of this result has resulted in the development of a simple Grignard-based addition to α -epoxy sulfonylhydrazones that provides exclusive *syn*-selectivity in the case of five and six-membered ring systems (seven membered rings and acyclic compounds will be examined in due course). A manuscript describing our preliminary data on the latter project is currently

been prepared for submission to *J. Am. Chem. Soc.* as a communication. As we had anticipated in our original proposal, both of the above methods allow an unusually broad range the alkyl groups to be incorporated into the α -epoxy sulfonylhydrazone substrates, including those having sp^3 , sp^2 , and sp hybridization. This has not previously been possible via a single method in the context of α -carbonyl-based functionalization.

The second line of research we have recently begun to investigate is the development of asymmetric Cu(I)-catalyzed addition of Grignard reagents to achiral azo-alkenes, using chiral nonracemic ligands. To date, three different ligands have been prepared, each involving a multistep synthesis. Using a model azoalkene, we have tested the addition of certain alkyl groups. At present, the highest level of enantioselectivity observed for these additions is 86:14. While an inspiring result, we are working to improve the selectivity through the design and synthesis of other chiral nonracemic ligands.

NICHOLAS K. CONRAD, I-1732, The University of Texas Southwestern Medical Center. BIOCHEMICAL ANALYSIS OF A NUCLEAR POLY(A)-DEPENDENT RNA DECAY PATHWAY.

In the nucleus of mammalian cells, RNAs are subject to degradation at nearly every step of gene expression. Despite their impact on gene expression, the mechanisms that cells use to degrade nuclear RNAs and the regulation of these pathways remains poorly defined. Our preliminary studies suggested that cells have a unique poly(A) tail dependent decay pathway dedicated to the degradation of nuclear polyadenylated transcripts. We proposed that this pathway is involved in RNA quality control by promoting the degradation of misprocessed RNAs and it may additionally be involved more directly in regulation of gene expression. Our major accomplishment this year has been to publish a paper (Bresson and Conrad, 2013) defining the major factors involved in this degradation pathway. These factors include the poly(A) binding protein, PABPN1, the poly(A) polymerases PAP α/γ and the nuclear exosome. Since the publication of this paper, we have made additional progress in understanding the requirements for PABPN1, PAP α/γ and the poly(A) tail in nuclear RNA decay and have surprisingly found a potential link between PABPN1 and gene transcription. In addition, we have continued our attempts to recapitulate these polyadenylation-dependent decay pathways *in vitro*, but have not yet found the appropriate conditions for this reaction. In the upcoming year, we will attempt to make progress in defining this pathway *in vitro* and to tease apart the roles of these factors in nuclear RNA decay and gene expression in general.

LYDIA M. CONTRERAS, F-1756, The University of Texas at Austin. *IN VIVO* STRUCTURE CHARACTERIZATION OF CATALYTIC RNAs BY FLUORESCENCE.

During our third year of funding (and third full year at UT), we have accomplished the following:

1. Optimization and testing of a second generation of probes (GenII) that span along the entire (~400nt gI intron RNA were characterized in terms of their sensitivity for structural detection and stability *in vivo* (alone and as complexes with the target). We have also tested the effect of binding energies and probe length. Lastly, we have confirmed that our optimized probes are capable of capturing both local structural differences as well as sequence mutations among different variants of the gI intron. These mutants include a catalytic mutant where minimum structural changes are expected and a quintuple mutant where major structural disturbances are expected.

2. Confirmation of our structural analysis with *in vitro* and *in vivo* DMS footprinting methods, now well established in our lab, and demonstration that our fluorescence-based approach poses advantages in identifying rarely observed folding intermediates among the gI folding pathway.

3. Design of a new system of probes to test if we can capture chemical modifications that affect RNA folding *in vivo* using a bacterial tRNA as a model system. These experiments are currently underway and will also explore our ability to probe RNA structures using natural cellular levels of a native RNA.

4. Confirmation that our probes are capable of picking up structural differences that arise from intracellular factors when RNA is folded *in vivo*. Currently, we have confirmed (previously reported) differences in the gI intron that take place *in vivo* as a result of the StpA chaperone factor. Following these preliminary results, we have constructed an entire transposon mutant library that is now being screened for additional factors that affect gI intron folding in bacteria.

5. Design and construction of a high-throughput version of our fluorescence-based assay, coupled to deep-sequencing technologies. Preliminary experiments have confirmed the feasibility of performing complete structural analysis of all local regions within an RNA in a single experiment.

6. Dissemination of this work as oral presentations at the American Institute of Chemical Engineering conference in November (in San Francisco) and at the American Chemical Society Meeting (ACS) in March of this year in Dallas. This work was invited to be presented at the 5th International Conference on Biomolecular Engineering.

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

1) We concluded several years of study of allele-selective inhibition of trinucleotide repeat gene expression by identifying allele-selective inhibitors of mutant atrophin-1 expression. These inhibitors belong to several different classes of chemically modified nucleic acids, including single stranded silencing RNA (ss-siRNAs, single stranded compounds that function through the RNAi pathway), unmodified duplex RNA, duplex RNAs modified with abasic residues, and duplex RNAs substituted with unlocked nucleic acid nucleotides (UNAs). We identified several compounds that were allele selective inhibitors of expression for three different trinucleotide repeat genes - huntingtin, ataxin-3, and atrophin-1. This finding suggests that it may be possible for a single therapeutic nucleic acid to treat multiple diseases and that there are several different chemical options for obtaining optimal nucleic acid agents.

2) We have developed a method for obtaining strand-specific small RNA libraries for RNA-SEQ that requires picograms of RNA. Key features include an intramolecular RNA circularization step to increase efficiency, a random priming step for full-length cDNA formation, and gel-free library purification. We used our protocol to generate a sequencing library from Argonaute 2 (AGO2) immunoprecipitated and UV-crosslinked (CLI P-seq) RNA

using amounts of material too low to be detected by standard methods.

3) The presence of RNAi factors like argonaute 2 (AGO2) in mammalian cell nuclei has been hotly contested. We showed that AGO2 and other factors are present in nuclei and are active towards nuclear RNA substrates.

4) Using our new RNAseq protocol we have investigated the identity of RNA species associated with AGO2 protein in human cell nuclei. We find many excellent candidates for interacting targets at RNAs that overlap gene promoters and RNA sequences near splice sites. A primary goal for 2014-2015 will be to investigate the biological relevance of these findings.

LUIS G. CUELLO, BI-1757, Texas Tech University Health Science Center. CRYSTALLOGRAPHIC AND FUNCTIONAL STUDIES IN KcsA-Kv CHANNEL CHIMERAS THAT DIFFER IN C-TYPE INACTIVATION PROPERTIES.

During this grant year, we have concentrated our effort to elucidate the molecular basis of the structural changes associated to C-type inactivation within the Kv channels selectivity filter (SF). To accomplish this goal, we have created a KcsA-Kv channel chimera by mutating the so-called KcsA's pore helix, which is behind the channel's selectivity filter and it is known to be crucial in determining the extent and rate of the C-type inactivation process, to make it very similar to the one found in the mammalian Kv-channel family. We have solved the crystal structure for the closed state of this chimera channel at atomic resolution (1.9 Å), which altogether with our previous crystal structures of KcsA trapped in different kinetic states allowed us to propose an atomic resolution interpretation for the gating process of the pore domain in K⁺ channels (manuscripts in preparation). This experimental achievement has placed us in a unique position to study the function and structure correlations of the pore domain of different Kv channels since currently we can study the structural and functional consequence of mutations around different type of chimera channel's SF and/or changing the ionic composition of the media i.e. to different alkali metal ions: K⁺ Li⁺, Rb⁺, Na⁺ and Tl⁺. Currently, we are in the process of obtaining the structures of this chimera channel in the closed state soaked in the above mentioned ions to correlate the structure and the function of the K⁺ channel pore domain when is moving these permeant ions.

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

Over-expression of MELK (residues 2-340) in *E. coli*, and its subsequent purification facilitated the development of a robust screening assay within the TX-SACT screening facility (the PI is the director of this facility). This allowed the identification of several potent (IC₅₀~50 nM) MELK inhibitors from a library of drug-like kinase inhibitors. We verified their mechanism of inhibition following resynthesis and enzymatic analysis. Recently, the structure of the catalytic domain of human MELK was reported. We have purified the human form suitable for structural analysis. We believe that by having potent lead molecules, as well as highly purified protein we are well-placed to embark upon a program of structure-based drug design to obtain potent (IC₅₀< 1 nM) and selective MELK inhibitors and test them in pre-clinical models.

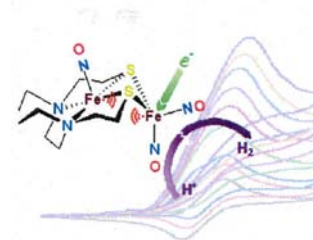
DONALD J. DARENSBOURG, A-0923, Texas A&M University. DESIGN AND REACTIVITY STUDIES OF METAL CATALYSTS FOR THE PRODUCTION OF POLYCARBONATES FROM NOVEL OXIRANES AND CARBON DIOXIDE.

Although cyclic carbonates have been shown to be the thermodynamic products of epoxide and CO₂ coupling reactions, the alternative kinetic copolymer product can be selectively generated if the growing polymer chain remains in contact with the metal catalyst during the process. This has been achieved by replacing the original binary (salen)metalX/onium salt catalysts by bifunctional (salen)metal complexes unsymmetrically substituted with an onium salt covalently attached to the salen ligand. These novel bifunctional catalysts have resulted in maintaining the growing anionic copolymer chain in close contact with the metal catalyst, hence preventing facile back-biting processes of the metal-free polymer chain leading to cyclic carbonate formation. Although these bifunctional catalysts are difficult to synthesize, we have developed an effective procedure for their synthesis, and continue to design other related, but more readily prepared, alternative catalyst systems. These new catalysts bear the covalently attached onium salt at the diamine functionality of the salen ligand.

Thus far, the bifunctional Co(III) and Cr(III) catalysts have made it possible for us to selectively synthesize several novel polycarbonates from the coupling of CO₂ and epoxides. New epoxides investigated successfully during the past year include: *cis*- and *trans*-2-butene oxide, isobutene oxide, cyclopentene oxide, 2-vinylloxirane, and 2,3-epoxy-1,2,3,4-tetrahydronaphthalene. A unique outcome of these studies is the observation that the copolymer derived from cyclopentene oxide and CO₂ can be catalytically depolymerized to its comonomers effectively under a reduced pressure, hence providing an ideal recycling pathway. This observation was suggested in advance based on our extensive computational studies of these CO₂/epoxide coupling reactions.

MARCEA Y. DARENSBOURG, A-0924, Texas A&M University. SYNTHETIC ANALOGUES AND REACTIVITY STUDIES OF IRON, NICKEL, AND ZINC BIOMIMETIC COMPLEXES CONTAINING HISTIDINE, CYSTEINE, AND NITRIC OXIDE AS LIGANDS.

As the area of bioorganometallic research progresses, the connection between low-valent iron in diatomic ligand settings such as the Fe(CO)₂CN unit in the hydrogenases and the Fe(NO)₂ unit in iron-sulfur cluster degradation of import to human physiology is of increasing interest. A broad collaboration connecting our synthetic expertise in the area of metallothiolates as ligands (M232, MS237) to such iron units with EPR and Mossbauer spectroscopists and electrochemists resulted in a clear delineation of the electrocatalytic proton reduction ability of redox-active iron nitrosyl units in a diiron complex whose core-structure is inspired by the [FeFe]-H₂ase active site (M233). The extent to which the iron atoms communicate in biomimetic diiron species is a question addressed by detailed Mossbauer spectroscopy where the magnetic hyperfine couplings for Fe(I)Fe(II) complexes derived from (μ-SRS)-[Fe(CO)₃]₂



precursors find non-equivalent sites of the oxidized species (M231). The discovery that $(\mu\text{-SRS})\text{-}[\text{Fe}(\text{CN})(\text{CO})_2]_2^{2-}$ can be inserted into the apo-H₂ase enzyme, has prompted revisiting the conformational mobility of $(\mu\text{-SRS})\text{-}[\text{Fe}(\text{CO})_3]_2$ and the effect of substituents on a pendent base, SCH₂NRCH₂S-, built into the p-SRS connector on electrochemistry and proton reduction (MA234). Other studies with this series found that N-substituted dithiolate bridges protected the diiron organometallics from oxygen degradation (MA235).

An intriguing hypothesis of CO/RS reductive ligand substitution from the last reporting period (M230) was developed as an $(x\text{-C}_6\text{H}_4\text{-S})(\text{NHC})\text{Fe}(\text{NO})_2$ series appropriate for mechanistic analysis by Hammett parameters (M.A.236), indicating that the Fe(NO)₂ electron density is a delocalized nucleophile in interactions with an incoming CO. The interesting possibilities for the Fe(NO)₂ as a unit for facilitating reactivity was also noted in the conversion of a metal-bound imidazole to the corresponding N-heterocyclic carbene ligand (M230).

OLAFS DAUGULIS, E-1571, University of Houston. NEW METHODS FOR CARBON-HYDROGEN BOND FUNCTIONALIZATION.

1. We have developed a method for direct, copper-catalyzed, auxiliary-assisted fluorination of $\beta\text{-sp}^2$ C-H bonds of benzoic acid derivatives and $\gamma\text{-sp}^2$ C-H bonds of α,α -disubstituted benzylamine derivatives. The reaction employs a CuI catalyst, a AgF fluoride source, and DMF, pyridine, or DMPU solvent at moderately elevated temperatures. Selective mono- or difluorination can be achieved by simply changing reaction conditions. This paper presents the first example of directed, copper-catalyzed fluorination of C-H bonds. It was highlighted in *C&E News* (2013, issue 26, p. 20).

2. Perfluorinated Cu-based metal-organic frameworks (MOFs) were prepared starting from extensively fluorinated biphenyl-based ligands accessed via C-H functionalization methodology developed in our group. These new materials are among the most water-repellent MOFs ever reported. This work is collaboration with Dr. Miljanic group at the University of Houston.

3. A unique ligand system based on 8-aryl-1-naphthylamine framework, accessed via our C-H functionalization methodology, was designed and tested in alkene polymerization. Catalysts derived from these ligands possess increased axial bulk relative to standard diimine-nickel complexes, resulting in lower rates of chain transfer relative to chain propagation rates and thus higher polymer molecular weights and narrower PDIs. They yield the most highly branched PE produced by Ni catalysts seen to date. Additionally, these catalysts are capable of chain-straightening polymerization of alpha-olefins. This work is collaboration with groups of Dr. Brookhart (UNC-Chapel Hill) and Dr. Coates (Cornell).

4. A method for direct, auxiliary-assisted alkoxylation and phenoxylation of $\beta\text{-sp}^2$ C-H bonds of benzoic acid derivatives and $\gamma\text{-sp}^2$ C-H bonds amine derivatives is reported. The reaction employs $(\text{CuOH})_2\text{CO}_3$ catalyst, air oxidant, phenol or alcohol coupling partner, DMF, pyridine, or DMPU solvent at 70-130 °C.

5. A method for base-promoted arylation of arenes and heterocycles by aryl halides and aryl triflates has been described. *In situ* electrophilic trapping of ArLi intermediates generated in the reaction of benzyne with deprotonated arenes or heterocycles has been developed, providing rapid access to a wide range of functionalized polyaryls.

JEF K. DE BRABANDER, I-1422, The University of Texas Southwestern Medical Center. NOVEL HETEROCYCLIZATIONS FOR NATURAL PRODUCT SYNTHESIS.

During the past grant year, we have made substantial progress on a variety of fronts, including the development of methodology for substructures relevant to medicinal chemistry programs, and the synthesis and biological evaluation of several natural products. In the area of heterocycle synthesis, we have developed novel methodology for the synthesis of 2-substituted dihydroquinoxalinones via a copper-catalyzed *N*-arylation of unprotected alpha amino acids with 2-iodoanilines followed by acid-mediated cyclodehydration of the resulting coupling products. Our method has the advantage over other methodology inasmuch that the mild reaction conditions enable coupling of a variety of arylglycines without epimerization/racemization at the amino acid chiral center. The resulting dihydroquinoxalinones are important subunits in a variety of biologically active drug candidates, for example in bradykinin receptor antagonists of importance for reversing chronic inflammatory pain. In the area of natural product synthesis, we have published two manuscripts related to the host factor targeted antiviral activity of our natural product analog Saliphenylhalamide. Finally, we initiated a total synthesis of a novel marine bacteria-derived natural product termed Mangrolide A, isolated by my colleague John MacMillan at UTSW. Mangrolide possesses potent Gram-negative selective antibacterial activity. Its structure consists of an 18-membered macrolactone decorated with an unusual disaccharide. We have synthesized several fragments of the mangrolide and are ready to begin explore coupling strategies during the next grant year.

RALPH J. DEBERARDINIS, I-1733, The University of Texas Southwestern Medical Center. GLUTAMINE-DEPENDENT REDUCTIVE CARBOXYLATION: A METABOLIC ACHILLES' HEEL IN CANCER.

Aim 1: We used metabolomics and metabolic flux analysis to identify several accessory metabolic activities required to drive glutamine-dependent reductive carboxylation (GDRC) in cancer cells. Our analysis surprisingly revealed that cells using reductive carboxylation to supply the lipogenic acetyl-CoA pool also undergo persistent partial oxidation of glutamine in the tricarboxylic acid cycle, producing a large intracellular pool of succinate. By silencing enzymes along this oxidative pathway, we determined that alpha-ketoglutarate dehydrogenase is required to sustain GDRC. Because this enzyme produces reducing equivalents as NADH, the data suggested a model in which partial glutamine oxidation generates reducing equivalents required to power the reductive carboxylation reaction. Additional gene silencing experiments confirmed and extended this model. Overall, the data revealed that GDRC requires branched metabolism of alpha-ketoglutarate, with oxidative metabolism supplying reducing equivalents which are transferred to NADPH by the enzyme nicotinamide nucleotide transhydrogenase, and ultimately consumed by isocitrate dehydrogenase-2 in the reductive carboxylation reaction. This work appeared

in *Cell Reports* in 2014.

Aim 2: We performed isotope tracing analysis in more than 80 lung cancer cell lines and ranked the cell lines according to their preference for GDRC. We then cross-referenced the metabolic data against gene expression and chemotherapeutic sensitivity data on the same cell lines in an effort to identify shared vulnerabilities among cell lines with a preference for GDRC. Unexpectedly, cell lines with the highest contribution of GDRC to overall TCA cycle flux shared a gene expression signature indicating an epithelial cell phenotype, and many contained activating mutations in the gene encoding the epithelial growth factor receptor (EGFR). Furthermore, there was a strong correlation across the panel of 80+ cell lines between GDRC and sensitivity to EGFR inhibitors. This is the first chemotherapeutic vulnerability associated with the GDRC metabolic phenotype.

GEORGE N. DEMARTINO, I-1500, The University of Texas Southwestern Medical Center. REGULATION OF PROTEASOME FUNCTION BY REVERSIBLE SUMOYLATION.

Consistent with the aims of the original proposal, we have established and characterized an *in vitro* system using purified proteins to reversibly modify the 26S proteasome with SUMO and to determine the functional consequences of this modification. We have covalently modified purified 26S proteasome with SUMO-1 using the SUMO conjugating enzymes SUMO E1, Ubc9, and PIAS-3. We have confirmed preliminary findings that the Rpn2 subunit of the PA700 regulatory subcomplex of 26S is modified with SUMO. Unexpectedly, we found that the Rpt2 ATPase subunit of PA700 is also covalently modified with SUMO-1. We have optimized conditions to maximize the extent of SUMO modification and isolated the SUMO-modified proteasome. Our analysis indicates that >75% of each subunit is SUMOylated, indicating that these modifications are not mutually exclusive. SUMOylation does not affect stability of 26S proteasome, measured by dissociation into 20S and PA700 subcomplexes, SUMOylation inhibited 26S proteasome activity against short synthetic peptides and against a model polyubiquitylated protein, (Ub)_n-Sic by more than 85%. Moreover, the ATPase activity of SUMOylated 26S proteasome was reduced by more than 90% compared to unmodified proteasome. These findings strongly support our preliminary data and original hypothesis. We are currently testing the effects of SENP1 on proteasome SUMOylation activities.

In an unexpected development, we have discovered that PI31, a protein inhibitor of the proteasome, blocks proteasome SUMOylation. We are currently investigating the mechanism of this effect. This finding raises the possibility that proteasome SUMOylation is regulated by multiple mechanisms and reveals a possible new function of PI31. We will extend this work to determine the role of PI31 on SENP1 action both *in vitro* and in cells.

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

We are exploring the late d-block element chemistry using highly fluorinated ligand versions of tris(pyrazolyl)borates and pyrazolates or weakly coordinating counter-anions like [SbF₆]⁻. Metal adducts of these "Teflon coated" ligands and weakly coordinating anions show unusually high thermal and air stability and very interesting chemical reactivity not usually seen with the related non-fluorinated analogs. During this project period, we reported the synthesis of some of the most weakly coordinating tris(pyrazolyl)borates and their silver alkene complexes. These silver adducts catalyze the insertion of carbene moiety from ethyl diazoacetate to C-H bonds of hydrocarbons very effectively. The related pyrazoles were used in the synthesis of copper and silver pyrazolates. They show luminescence and form supra-molecular aggregates with interesting structural features. Widely available [SbF₆]⁻ counter ion and N-heterocyclic carbene ligand were used in the stabilization of first gold(I) complexes of organic azides. Their nitrogen extrusion chemistry was probed in detail. We have also isolated and investigated the chemistry of carbonyl and isocyanide adducts of copper on a bis(cyclooctyne) template. These [CuL₂L']⁺ adducts feature spoke-wheel structures.

MICHAEL R. DIEHL, C-1625, Rice University. ACTIVATED SPATIAL REGULATION OF INTRACELLULAR CHEMISTRY.

We have demonstrated unique abilities to configure the expression level, localization and mobility of interacting / networked proteins within living cells. This advance is highlighted in our report [Efremov *PNAS* 2014] that employed synthetic and biophysical approaches to control and examine the passive and activated motile properties of vesicular organelles, key carriers of signaling enzymes and substrates. We have also built upon these capabilities by developing new regulatable protein expression constructs that possess custom-tailored expression responses to enable the selective and robust targeting of proteins to specific sub-cellular compartments [Kumar et al, in preparation]. Our new expression systems utilize negative feedback circuitry and exhibit exceptionally low expression noise and heterogeneity among cells populations. We have also generated large, multi-gene systems that provide unique abilities to regulate the expression of multiple distinct proteins simultaneously and have established robust methods to prepare isogenic populations of cells incorporating these integrated gene systems. The successful development of these tools has also allowed us to overcome key challenges associated with utilizing light-dependent protein dimerization switches to tune protein localization and mobility. Together, these advances now provide a powerful foundation to configure the status of synthetic multi-enzyme networks that can function as experimental models to explore how expression level, localization, diffusion and transport impact the composite responses of protein networks in living cells.

GUANGBIN DONG, F-1781, The University of Texas at Austin. SITE-SELECTIVE C-H BOND FUNCTIONALIZATION.

A. In search for a *ketone-directed C-H functionalization*, we first developed a Pd-catalyzed direct β -arylation of ketones using aryl halides (Eq 1). Simple cyclic ketones with different ring-sizes, and acyclic ketones can be directly arylated at the β -position with complete site selectivity and high functional group tolerance.

B. Aiming to alkylate ketones using simple unactivated olefins (alkynes/allenes), we have proposed a transition metal and amine-cocatalyzed C-H functionalization strategy. This strategy is expected to 1) *substitute expensive and toxic halogen reactants with cheap, more environmentally benign olefins*; 2)

allow reactions to occur at neutral and catalytic conditions without stoichiometric strong bases; 3) offer a byproduct-free process. Recently, we achieved breakthroughs on alkylating normal ketones (i.e. cyclopentanones or acetones) with *simple olefins or alkynes* by employing new catalysts (Eq 2).

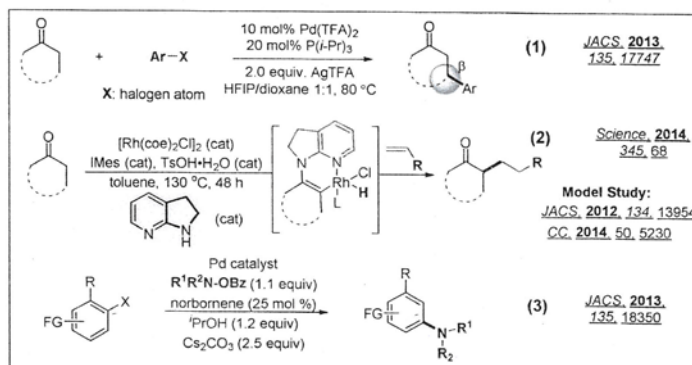
C. We developed a Catellani-type vicinal C–H amination reaction of arenes with a broad scope and functional group compatibility, which provides complementary site-selectivity from Buchwald–Hartwig aminations (Eq 3).

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

The transcriptional program of HIV relies on the transcription factor Tat, which recruits the cellular transcription elongation factor P-TEFb formed on viral nascent pre-mRNAs at the HIV promoter. We previously found that P-TEFb is recruited at the HIV promoter as part of the inhibitory 7SK snRNP complex, which inactivates its kinase activity. However, it has long been unclear how Tat captures P-TEFb from this complex to stimulate P-TEFb kinase activity and transcription elongation. We have recently proposed the mechanistic basis by which Tat mediates the enzymatic release of P-TEFb from the 7SK snRNP at the viral promoter to trigger gene activation. We demonstrate that Tat recruits PPM1G/PP2Cg to locally disassemble P-TEFb from the 7SK snRNP at the HIV promoter via dephosphorylation of the kinase T loop. Interestingly, we found that this hijack mechanism is also utilized by the cellular transcription nuclear factor (NF)- κ B. Similar to Tat, NF- κ B recruits PPM1G in a stimulus dependent manner to activate elongation at inflammatory-responsive genes. Recruitment of PPM1G to promoter-assembled 7SK snRNP provides a paradigm for rapid gene activation through transcriptional pause release. Ongoing experiments will enable us to dissect out the precise mechanism by which P-TEFb/7SK snRNP is directly recruited to chromatin to regulate Pol II transcription elongation, as this step could be targeted to precisely block transcription chemically.

MICHAEL DOWNER, F-1038, The University of Texas at Austin. FEMTOSECOND NONLINEAR SPECTROSCOPY OF COLUMN IV NANO-INTERFACE CHEMISTRY.

Our Welch-sponsored research focuses on characterizing bond structure and chemical interactions at semiconductor nano-interfaces using noninvasive optical probes. Complementing previous Raman spectroscopy studies and motivated by bio-sensing applications, we have demonstrated efficient two-photon femtosecond excitation of photo-luminescence from ligand-stabilized, water-soluble Si nanocrystals (NCs) in the tissue transparency spectral window. Quantitative studies are continuing. Following up on the noninvasive, but spatially-averaged, scanning second-harmonic generation (SHG) method for characterizing performance-limiting anti-phase domain (APD) defects in GaAs films on Si substrates, reported last year, we have now resolved *individual* APDs of 0.1 micron lateral size by developing SHG near-field scanning optical microscopy (NSOM). In collaboration with colleagues in UT's College of Engineering, we have also obtained initial SHG scanning microscopy results from asphalt binders, to detect self-healing cracks, and from novel A-site-ordered double perovskite microcrystals, to confirm ferroelectricity in a new class of ferro-electrics. In a new initiative, we developed single-shot ultrafast methods for imaging nonlinear propagation of femtosecond laser pulses through gaseous [*Opt. Lett.* **38**, 5157 (2013)] and solid [*Nature Commun.* **5**, 3085 (2014)] Kerr media, thereby visualizing laser filament dynamics that underlie remote atmospheric chemical analysis and micromachining. Contributions of atmospheric molecular rotations to the Kerr effect were spatially and temporally resolved.



REBEKAH DREZEK, C-1598, Rice University. PREPARATION AND CHARACTERIZATION OF GOLD NANOPARTICLES (AuNPs) USING CO REDUCTION.

Our work has focused largely on developing approaches to improving gold nanoparticle synthesis as applied to particles with near infrared optical response. A paper recently published online in *Particle* describes one new approach to this challenge developing nanoparticles using sub-30 nm gold chalcogenide cores decorated with Au islets, which provide tunability from the visible to SWIR in a small particle size suitable for biological application and are not dependent on a full metallic shell adding significant flexibility. A second paper recently accepted to *Nanoscale* describes a particle structure consisting of a plasmonically active hollow gold nanoshell core surrounded by photoluminescent quantum nanocrystals (QNs) encapsulated by a silica layer. The paper describes synthesis of the complex and demonstrates an approach to monitoring temperature changes through changing photoluminescent properties. Both papers take advantage of much of the synthesis described in the *Nanoscale Research Letters* paper on AuNP synthesis using CO reduction we reported in a prior Welch report

RUI-RUI DU, C-1682, Rice University. INFRARED AND MICROWAVE SPECTROSCOPY OF GRAPHENE AND 2D TOPOLOGICAL INSULATORS.

1. We have made an instrumentation of co-planar waveguide microwave resonant circuit, by which we are planning to measure the helical edge modes of quantum spin Hall insulator in InAs/GaSb quantum wells.

2. In collaboration with IBM group, we observed edge transport in the topologically insulating InAs/GaSb system where electronic transport properties were influenced by certain disorder scatterings. The results show that conduction occurs exclusively along the device edge. Both quantized and self-averaged transport shows resilience to magnetic fields.

3. The edge currents in the InAs/GaSb topological insulator were imaged by a collaboration of Rice and Stanford groups. A major finding is that, although the effective edge resistance is much greater than resistance quantum, it is independent of temperature up to 30 K. Known candidate scattering mechanisms do not explain our observation.

KIM R. DUNBAR, A-1449, Texas A&M University. MAGNETIC AND ELECTRONIC PROPERTIES OF MOLECULAR MATERIALS: INVESTIGATION OF FACTORS THAT EFFECT BISTABILITY.

In this last project period, our modular approach to designing homologous series of compounds has led to families of structurally related molecules with the same geometrical arrangement of spin centers; this approach will continue to be exploited in the next year. Armed with the successful elaboration of record magnetic coupling and blocking temperatures for cyanide-based SMMs, we are poised to further advance fundamental knowledge about how single-ion anisotropy profoundly manifests itself in terms of magnetic bistability. We continue to be interested in early transition metal ions from groups five and six that have been very little explored or entirely unexplored in cyanide chemistry. We are also targeting families of mononuclear compounds of transition metal and lanthanide ions that display bistability (they behave as miniature magnets) in spite of the few number of spins that they possess, a topic that is growing quite rapidly in the literature. The concept of using organocyanide radicals as bridges for SMMs is one that we introduced to the community a number of years ago and recent results from this Welch grant have led to exciting new hybrid magnetic conductors which are of an unprecedented type. We have also delved more deeply into the issue of how geometry and metal ion single-ion anisotropy affect the magnetic properties of related families of molecules. Much of the direction is inspired by exciting recent findings including our successful preparation of a mixed Mo_2V_3 molecule with a record exchange coupling through the cyanide ligand and an SMM with a record barrier and hysteresis for a cyanide compound based on Mn_2Mo which are important experimental evidence that theorists are doing an excellent job of pointing chemists in the right direction. Another major unpublished result in the past few months is our synthesis of the first example of a heptacyanotungstate anion, a finding that presages a future of exciting new studies for 5d metal ion cyanide magnetism.

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

Electron transfer in collisions between potassium atoms in high Rydberg states and targets that attach free low-energy electrons is used to create molecular ion-pair states (denoted by $X^+..Y^-$ or $X^+..YZ^-$) in which a positive-negative ion pair orbit at large separation weakly bound by their mutual Coulomb attraction, also termed heavy-Rydberg ion-pair states. A new apparatus in which the region where the ion-pair states are formed is separated from that in which they are analyzed has been commissioned to study their formation and their chemical and physical properties. The angular and velocity distributions of the product ion-pair states are determined using electric-field-induced dissociation to examine how these depend on the parent Rydberg state and the reactant velocities. Ion-pair lifetimes are being measured to study their destruction through processes such as mutual neutralization via charge exchange and the conversion of internal energy in the anion into translational energy of the ion pair. Studies with strontium Rydberg atoms have shown that much higher Rydberg production rates can be achieved than obtained when using potassium. Since their use will dramatically increase the data rates in our ongoing experiments and will allow study of effects associated with excitation of the (positive) core ion, we are upgrading the apparatus to use strontium. Work is also in hand to manipulate the electron spatial and momentum distributions in the parent Rydberg atoms to better control the initial formation conditions.

RON ELBER, F-1783, The University of Texas at Austin. PASSIVE TRANSPORT THROUGH MEMBRANE.

We develop theories and computer programs to simulate the transport of moderately sized molecules through membranes. In the past year we focused on better understanding long time density fluctuations and thermal motions of lipid bilayers and their impact on permeation of molecules with variable sizes. The membrane is presented by a density field, the number of atoms of a particular type in a volume element. We probe the transition between different values of the density in atomically detailed simulations and construct a kinetic model for these transitions. To investigate transport phenomena one of the field densities we defined was that of water molecules. We asked what is the probability to observe a particular water density within the membrane and ultimately what is the probability of having water molecules transported directly and passively through membrane. We also computed the time scale of water translocation. We further investigated the mechanism of this transport; this turned out to be novel and intriguing. In contrast to earlier studies of water permeation that assumed a single coarse variables (the position of the transported water molecule along the axis normal to the membrane plane), we searched for alternatives or additional variables and found that the permeating water molecule does not like to act alone. The permeation progresses efficiently when the water molecules form a cluster with a monotonic decreasing size as a function of the membrane depth. The water cluster size is at a minimum in the center of the membrane. However, at no point is the permeation of an isolated water molecule. At the center and the top of the free energy barrier the cluster is of two water molecules. The second order parameter is the density of water molecules. We have shown that the reaction coordinate is highly curved in the combined space of cluster size and membrane depth. Finally the free energy of cavity formation in membranes correlates well with the free energy of embedding hydrophobic molecules in membranes. An example is a xenon atom.

ANDREW D. ELLINGTON, F-1654, The University of Texas at Austin. THERMOSTABLE T7 RNA POLYMERASE FOR DIAGNOSTIC APPLICATIONS.

As noted in the report from the previous year, we have achieved success in applying our novel system for directed evolution, CPR, to the evolution of T7 RNA polymerase promoter specificity. In the past year, we have expanded upon this success and generated a panel of six highly active and specific polymerase: promoter pairs, which are currently being used to create complex genetic circuitry.

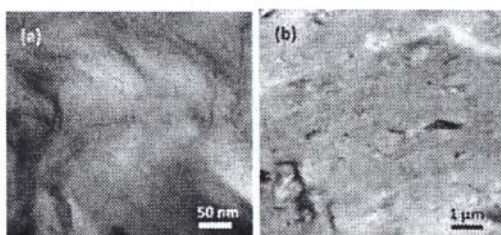
We have also used a rational engineering approach to combine mutations thought to stabilize T7 RNA polymerase with mutations known to alter substrate specificity (which we hypothesized destabilized the polymerase). The addition of stabilizing mutations to substrate specificity mutants does not appear to alter their specificity, but markedly improves their overall activity. This advance facilitates the creation of unnatural RNA in high yield, which had previously not been possible. These mutants are currently being used by several labs to allow for the *in vitro* selection of functional RNAs with unnatural bases.

To build upon this success we have taken a directed evolution approach, using CPR to remake the active site of T7 RNA polymerase, thus further enhancing its ability to accept unnatural substrates. We are also using CPR to form a "neutral drift" library of T7 RNA polymerase variants. In this endeavor, T7 RNA polymerase is selected for its normal function, but under an extremely high mutation rate. As most mutations are destabilizing, the polymerase is forced to evolve compensatory stabilizing mutations in order to survive. Our resulting population contains several mutations found in at high frequency, which presumably help to stabilize the polymerase, and have never been reported in the literature. Work is ongoing to determine the exact nature of these mutations. These mutations may be useful in the creation of thermostable polymerases, or to enhance the activity of substrate specificity mutants. The neutral library itself can also serve as the starting point for selections for phenotypes that are poorly understood and likely require multiple mutations spanning the entire molecule (e.g. processivity).

CHRISTOPHER J. ELLISON, F-1709, The University of Texas at Austin. CHEMISTRY AND PROPERTIES OF SELF-ASSEMBLY DIRECTED NANOMATERIALS.

In the past year, new progress has been made in understanding the hierarchical structure of the clay-poly (octadecyl acrylate-block-styrene) (MMT-PODA-b-PS) block copolymer (BCP) nanocomposites. Strong interactions between the clay sheets and BCP matrix chains, even at high clay content (> 10 vol%), were found to enhance the degree of clay exfoliation as shown in the TEM images in Figure (a) and (b) at two different magnifications. Remarkably, we also discovered a 300% increase in crystallinity formed by the side chains of the PODA block compared to their free BCP counterparts. This is true of many different samples synthesized as a "library" of materials and is proof that our synthesis approach enabled us to obtain densely grafted blocks which formed highly stretched PODA backbones, leading to the enhanced alignment of the side chains and higher crystallinity.

These materials were also cast into films of different thickness, and they demonstrated very high optical transparency. For example, a 6.2 μm thick nanocomposite film had an average transmittance of 92.3% across the entire visible light spectrum, which is nearly 20% higher than previously reported nanocomposite films. This suggests potential coating or packaging applications which require high optical clarity and good gas barrier properties. Future work for this project will involve a more detailed study of the morphological behavior of the surface-grafted BCP matrix to fundamentally understand the structural implications of surface tethering self-assembling chains on a high aspect ratio nanosheet.



STEFAN K. ESTREICHER, D-1126, Texas Tech University. DYNAMICS OF IMPURITIES IN SEMICONDUCTORS.

The accepted reason why defects lower the thermal conductivity of materials is that thermal phonons somehow scatter off defects which in turn reduces the flow of heat. We have developed a strictly microcanonical scheme to perform *ab-initio* non-equilibrium MD simulations with unprecedented temperature control (temperature fluctuations as low as $\pm 1\text{K}$ at 125K). These calculations allow us to prepare a supercell slightly away from equilibrium, and then monitor the energies and amplitudes of all the normal vibrational modes vs. time. The results show that (1) all defects introduce (low- and high-frequency) modes that are localized in space; (2) thermal phonons trap in these modes; and (3) the vibrational lifetimes of defect-related modes are one- to two-orders of magnitude longer than those of bulk phonons of the same frequency. Thus, we find that defects lower the thermal conductivity because they trap small amounts of energy for some length of time - not because they scatter phonons. Phonon trapping does not conserve momentum. Indeed, after dozens or hundreds of periods of oscillation, the origin of the excitation is forgotten. Thus, phonon-defect interactions have nothing to do with scattering. Further, the decay of trapped vibrational excitations depends only on the availability of receiving modes, and this suggests that heat flow could be controlled using specific interfaces. Ongoing research involves the interactions of between heat flow in a Si nanowire and a 6-layer of C (or Ge), which has higher- (or lower-)

frequency modes than Si. The phonons trapped at the Si/C (or Si/Ge) interface should decay back into Si (or into Ge) resulting in a large effective coefficient of reflection (or transmission). Quantifying such coefficients at the *ab-initio* level raises all sorts of challenges.

Research on 3d transition metal impurities in Si is nearing its conclusion. We have predicted that the diffusivities of interstitial Cu and Ni in Si should be much larger than the accepted literature values and these predictions have been confirmed by new experimental studies. Ongoing work involves Zn, for which little information is available.

DONGLEI L. FAN, F-1734, The University of Texas at Austin. INVESTIGATION OF A GENERAL MECHANISM FOR RATIONAL SYNTHESIS OF THREE-DIMENSIONAL SEMICONDUCTOR NANOSUPERSTRUCTURES BY DESIGNED CHEMICAL CATALYSTS.

3-D porous Cu-Ni superstructure catalysts were rationally designed and synthesized by strategically porosifying commercially available 3-D Ni foams via an alloying-etching approach. The approach consists of three steps: firstly, an alloying element, such as Cu, was conformably coated on the entire surface of 3-D Ni foams by electrodeposition. Then, the Cu-Ni composite was annealed (1100°C) for interfacial atomic diffusion and alloying. Next, the Cu element was selectively etched from the Cu-Ni alloy foam by electrochemistry. As a result, arrays of micropores of ~5 μm can be formed on the 3-D microbranches (100 μm) of Cu-Ni foams. Using this method, more than two-thirds surfaces of Ni foams can be porosified. The total surface areas of the 3-D catalysts can be readily increased by two times. The pore morphology, size, and density can be controlled by the applied potential, etching rate, PH values, reaction time, and temperature. The detailed mechanism is under investigation.

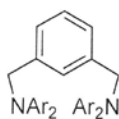
Employing the 3-D metallic catalysts with (and without) multilevel porosities, we synthesized two types of materials for energy storage devices: (1) semiconductor cobalt oxide nanowires. Dense arrays of cobalt oxide nanowires can be formed conformably on the 3-D catalysts. We applied them as electrodes for the lithium air batteries by collaboration with Prof. Manthiram. The devices show enhanced performances in our preliminary study. (2) 3-D multilevel porous graphene/thin graphite. The lattice fringe in HRTEM, small D band in Raman spectrum, and sharp peaks in X-ray diffraction (XRD) suggest the high crystallinity of the graphene/graphite. We further synthesized Ni(OH)₂ nanoplates and Mn₃O₄ nanospheres on the as-obtained 3-D thin graphite for applications in batteries and supercapacitors and achieved performance of ~480 mAh/g and ~3962 F/g at a discharging rate of 1.5 A/g, respectively, which are among the best compared to the previous reports.

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

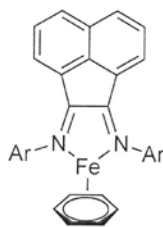
We extended our work developing reversible covalent enzyme inhibitors (*ACS Chem Biol* paper) to explore structure and inhibition of a boronate series and found that some compounds unexpectedly access a second binding pocket (manuscript in preparation). We have also extended this work by preparing a fully-active circularly permuted form of the protein, which enables us to make inactive, yet fully "matured" variants that we are now using to trap and structurally characterize bound substrates. We believe this is an innovative way to combine protein engineering and probe design. We also continued development of covalent probes for human dimethylarginine dimethylaminohydrolase (DDAH), describing a potent biologically-active inhibitor and the upregulation of this enzyme in 80% of melanomas (*ChemMedChem* paper). We extended this work by dissecting the probe into fragment-sized pieces and reassembling with a lengthened linker, resulting in the most potent inhibitor for this enzyme to date (manuscript in preparation), for which we demonstrated in-cell activity using a cell-permeable clickable activity probe. We also extended our discovery of halopyridines as selective covalent protein modifiers and are revising a paper on this for resubmission to *J. Am. Chem Soc* as a full paper instead of a communication. Finally, we discovered a covalent inhibitor for the antibiotic resistance determinant New Delhi Metallo-beta-lactamase- 1 (NDM-1) and found that a conserved active-site Lys residue can be selectively modified. Development of covalent probes for biological catalysts continues to be a fruitful area of study and will continue in the following grant period.

MICHAEL FINDLATER, D-1807, Texas Tech University. BASE METAL CATALYZED OLEFIN METATHESIS REACTIONS.

The proposal for this grant outlined the following for 2013-2016: 1) synthesis and characterization of ligand scaffolds capable of supporting reactive iron centers and metallation of those ligands; 2) preliminary studies of olefin metathesis activity employing cycloolefins as substrates; 3) isolation of a terminal iron-alkylidene. The last year has seen impressive strides in our research plans. As per the proposal, we have already completed the synthesis of aryl-substituted NCN ligands (**A**). The syntheses of N-aryl substituted ligands of this type are not trivial and, despite being a "textbook" reaction, were previously unreported or occurred only in poor yields. Thus, we devoted considerable time and effort to optimize a synthetic pathway, which was easily scalable, to provide facile access to ligand type **A**. This work was published in *Synthesis* this year. We are currently in the process of optimizing metallation conditions for this ligand set. We have successfully completed the synthesis of iron-complexes of type **B** and are exploring, per the proposal, methods of displacing the bound arene with neutral two electron donors. Thus far, we have been able to substitute the arene with carbon monoxide, use of highly fluorinated arenes should allow displacement with weaker carbene ligands. A manuscript describing this chemistry is currently in preparation and will appear in the upcoming grant year. Unexpectedly, and as the result of Welch support, we have discovered a new C-C bond forming reaction, which reductively couples olefins with olefins and olefins with aldehydes. This work has been submitted for publication. Over the last 12 months, Welch support has led to one published article, one submitted for publication and two more planned in the near future.



A



B

ILYA J. FINKELSTEIN, F-1808, The University of Texas at Austin. MOLECULAR MECHANISMS OF REPLICATING THROUGH DNA LESIONS.

Since the start of the grant period, we developed and published a method to enable molecular biology labs—even those lacking access to nano-/micro-fabrication equipment—to rapidly construct sophisticated microfluidic devices (Robison & Finkelstein, *Analytical Chem*, 2014; Robison and Finkelstein, *FEBS Lett*, 2014; Sipvey et. al., *Analytical Chem*, 2014). We also integrated microfluidics into our single-molecule "DNA curtain" imaging platform. Although DNA curtains increase the number of molecules that can be imaged in a single reaction, numerous independent experiments are still required to systematically map out all relevant reaction conditions (e.g., nucleotide state, salt concentration, or protein composition). Microfluidic device integration offers a powerful opportunity to further expand the capabilities of the DNA curtain platform. For example, by constructing a five-channel linear gradient generator, we can concurrently observe up to five distinct biochemical reactions on the same chip and will permit us to rapidly characterize key aspects of the T4 replisome activity at the single-molecule level.

In addition, we purified and biochemically characterized all eight proteins that are required to assemble the T4 replisome. We optimized conditions for assembling the T4 replisome and have set up a rolling circle replication assay (RCR) for biochemically characterizing wild type and fluorescently-labeled protein constructs. By using this assay, we identified fluorescent replisome proteins (e.g., the processivity clamp gp45[E212C]) that maintain full biochemical activity. Ongoing work is aimed at establishing a single-molecule fluorescence-imaging assay for T4 replisome activity.

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

Understanding the mechanisms by which the pterin-dependent non-heme iron enzymes activate oxygen has proved challenging because of the active Fe(II) enzyme is EPA-silent, and there is no chromophore to monitor during the reaction. We have been using NO as an oxygen mimic to generate EPA-detectable species. This has allowed us to detect changes in the active site as the substrates tyrosine and tetrahydrobiopterin bind. Hyperfine sublevel correlation and two dimensional electron spin echo analyses have been carried out of NO complexes in the presence and absence of the substrates. The results are consistent with two water molecules as iron ligands in the complex with tyrosine alone. Upon formation of the complex with both tyrosine and tetrahydrobiopterin, a model for the reactive oxygen-containing complex, the waters dissociate and both carboxylate oxygens of Glu376 coordinate the iron, resulting in a 5-coordinate complex. The Fe-NO bond points toward the aromatic side chain of the substrate tyrosine in the binary complex but has reoriented toward the pterin in the ternary complex. We previously showed that the E332A mutant enzyme reacts with oxygen but does not form the Fe(IV) hydroxylating intermediate; the tetrahydropterin is oxidized directly to dihydropterin. Characterization of the mutant protein shows that it can form the reactive complex. We attribute the lack of a productive reaction in the mutant protein to destabilization of the complex due to the loss of the interaction between Glu332 and the pterin.

CHARLES M. FOLDEN, III, A-1710, Texas A&M University. FIRST CHEMICAL INVESTIGATION OF ELEMENT 113.

Significant progress was made during the previous grant year. Our group continued to characterize and improve the extraction efficiency of a "gas stopper" that was described in the previous progress report. This device collects the products of nuclear reactions and makes them available for chemical experiments. A major experiment in March 2014 showed that the device has an efficiency of up to $(70 \pm 9)\%$ under optimum conditions, which is close to the world record efficiency. The device is capable of extracting either short-lived or long-lived radionuclides, and produces a low-emittance beam which may make it suitable for future experiments requiring precise ion injection, such as a quadrupole mass spectrometer. A publication on this work is in the very late

stages of preparation. Additionally, a new post-doctoral researcher, Dr. Evgeny E. Tereshatov, joined the project, and is working to identify chemical systems for group 13 elements which could be used in a first chemical experiment on element 113. Preparatory experiments will study the extraction behavior of its lighter homologs In and Tl under ultra-trace conditions, and Dr. Tereshatov has identified ^{111}In (half-life 2.80 d) and ^{202}Tl (12.31 d) as the most promising isotopes for homolog experiments. First production runs for these isotopes are expected in 2015. Finally, graduate student Ms. Marisa C. Alfonso completed her work on ultra-trace extraction of Zr and Hf from commercially available resins. A publication on this work is in the early stages of preparation, and she expects to earn her Ph.D. in December 2014.

MATTHEW S. FOSTER, C-1809, Rice University. TOPOLOGICAL MATTER PHASES UNDER EXTREME DURESS: DYNAMICS AND DISORDER.

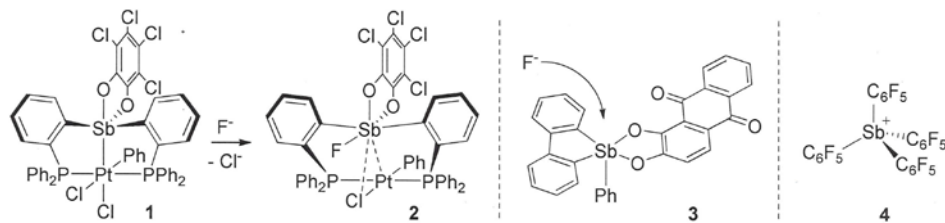
Both objectives outlined above were fully accomplished, and led to a series of publications with significant results. First, we showed that an ultracold fermion gas driven far from equilibrium can exhibit gapless Majorana edge modes (the hallmark of a topological superfluid). We showed that one must distinguish two different notions of topology, that of the state, versus that of the synthetic spectrum of excitations above the non-equilibrium state. Most important, we demonstrated that a quantum quench can be used to produce a "Floquet" topological superfluid in an ultracold gas of ^{40}K or ^6Li with non-equilibrium oscillations of the order parameter (superfluid Higgs mode) that should be detectable in experiment. This is a crucial advance, because parasitic effects make the adiabatic stabilization of equilibrium topological superfluids in these gases unfeasible. All of these results are asymptotically exact at long times (before parasitic effects kick in), and were obtained analytically, exploiting the integrability of the p-wave BCS Hamiltonian. There is now an intense experimental search to identify bulk solid state topological superconductors. We demonstrated that the Majorana surface states of such systems are robust to the effects of disorder and weak interactions, treating the effects of disorder exactly with conformal field theory, and interactions non-perturbatively in a large topological winding number expansion. Most important, we showed that the surface spin and thermal conductivities are unmodified by either disorder or interactions at low temperatures, and are topologically quantized. This should provide a "smoking gun" for experimental detection.

DOUG E. FRANTZ, AX-1735, The University of Texas at San Antonio. DEVELOPMENT OF NON-TRADITIONAL CATALYTIC PATHWAYS OF STEREODEFINED ENOL TRIFLATES.

We are pleased to report that our preliminary experiments to promote the interception of an intermediate palladium π -allyl complex generated from (*E*)-enol triflates with several heteroatom-based nucleophiles have been very successful. Key to the success of these preliminary reactions is the identification that *N*-heterocyclic carbene (NHCs) ligands on Pd appear to be the ideal ligands to catalyze the tandem sequence of oxidative addition/ β -hydride elimination/hydropalladation that generates an intermediate Pd- π -allyl complex. In turn, this complex is long-lived enough to be intercepted with several heteroatom nucleophiles including phthalimides, phenols, and most recently azide. More importantly, we have been able to fine-tune the reaction conditions through ligand optimization to provide the linear products in high selectivities over the branched products. We are confident that the culmination of these studies will be reported in the near future providing the synthetic community with an orthogonal yet complementary approach into electrophilic Pd- π -allyl complexes.

FRANÇOIS P. GABBAÏ, A-1423, Texas A&M University. CATIONIC GOLD-ANTIMONY COMPLEXES- LEWIS ACIDIC AND CATALYTIC PROPERTIES.

As part of our interest in the chemistry of dinuclear cationic complexes featuring an antimony(V) moiety, we have investigated the structure and properties of the tetravalent platinum stiboranyl complex $[(o\text{-}(\text{Ph}_2\text{P})\text{C}_6\text{H}_4)_2(o\text{-}\text{C}_6\text{Cl}_4\text{O}_2)\text{Sb}]\text{PtCl}_2\text{Ph}$ (**1**) (*Angew. Chem. int. Ed.* 2014, 53, 2633). Reaction of this compound with fluoride triggers an internal redox reaction which affords the fluorostiborane platinum(II) complex **2**. This reaction, which illustrates the high fluoride affinity of the stiboranyl ligand of **1**, is accompanied by a cleavage of the covalent Pt-Sb bond present in **1** and formation of a longer and weaker Pt \rightarrow Sb interaction in **2**. In parallel to this work, we have investigated the fluoride anion affinity of other pentavalent antimony species and have discovered that simple stiboranes such as **3** can be used for the fluorescence turn-on sensing of fluoride anions in aqueous media (*Chem. Sci.* 2014, 5, 1886). Finally, we have recently described the perfluorinated stibonium cation $[\text{Sb}(\text{C}_6\text{F}_5)_4]^+$ (**4**), a potent Lewis acid which abstracts a fluoride anion from $[\text{SbF}_6]^-$ and $[\text{BF}(\text{C}_6\text{F}_5)_3]^-$, indicating that it is a stronger Lewis acid than both SbF_5 and $\text{B}(\text{C}_6\text{F}_5)_3$ (*J. Am. Chem. Soc.* 2014, 136, 9564). This unusual cation, which has been isolated as an air-stable $[\text{B}(\text{C}_6\text{F}_5)_4]^-$ salt, polymerizes THF and promotes the hydrodefluorination of fluoroalkanes in the presence of Et_3SiH .



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

We have made significant progress in the last year on developing and applying simulation tools to address the connections between the self-assembly and properties of mixtures of organic and inorganic molecules. An area we have specifically targeted in the last year is the phase behavior of block copolymer and polymer blends possessing conjugated groups and hence a natural conformational rigidity. We have demonstrated that the use of a combination of polymers which contain such groups may lead to unique self-assembled structures which possess properties desirable for applications in the context of organic photovoltaic devices. In other contexts, we studied the ionic conductivity characteristics of polymer based electrolytes and demonstrated that a strong correlation between the ion mobilities and the corresponding conformational dynamics of the polymer molecule. A third line of our work has continued our fundamental quantum mechanical and coarse-grained simulations based modeling of the transport of ions, molecules and protons through a variety of polymeric membrane materials. Our researches were in collaboration with Chemists and our simulations provided valuable insights in rationalizing some intriguing experimental observations.

KEVIN H. GARDNER, I-1424, The University of Texas Southwestern Medical Center. COMPARATIVE STUDIES OF THE SIGNALING MECHANISMS OF FLAVIN-BASED PROTEIN PHOTOSENSORS.

Light is arguably the most universal environmental factor for biology, controlling growth, movement and metabolism in almost every organism on Earth. Such control requires photosensory proteins, tuned to convert different wavelengths of light into conformational changes that alter the function of downstream signaling proteins. Complementing these natural uses, an increasing number of novel "optogenetic" applications depend on engineered variants that provide researchers with unparalleled control of many types of *in vitro* and cellular chemistry. Mechanistic knowledge of photoreceptors enables the tuning these proteins, which is essential to their applied uses. Over the past year, we have focused on mechanistic studies of LOV (Light-Oxygen-Voltage) blue light photosensors, one of the broadest groups of such proteins. Our work has centered on two classes of bacterial LOV proteins: 1). light-activated DNA binding proteins (Zoltowski *et al.*, 2013), providing the foundation for tools which let researchers specifically control levels of gene expression in cells with simple blue light illumination (Motta-Mena *et al.*, 2014); 2). light-dependent two-component signaling systems (Correa *et al.*, 2013), a member of the most common kind of bacterial environmental sensor. Our research has revealed a long-sought high-resolution atomic structure of this sensor (Rivera-Cancel *et al.*, 2014), providing both basic mechanistic insights and inspiration for novel approaches to use these enzymes in novel biotechnology applications.

WILLIAM T. GARRARD, I-0823, The University of Texas Southwestern Medical Center. FORMALDEHYDE CROSS-LINKING FOR DISCOVERY OF NOVEL REGULATORY ELEMENTS EXHIBITING LONG-RANGE INTERACTIONS WITHIN AND BETWEEN CHROMOSOMES.

To understand the relationships between nuclear organization and gene expression in a model system, we employed 3D-imaging and ChIP-3C techniques to investigate the topographies of the immunoglobulin (*Ig*) genes and transcripts during B cell development. Remarkably, in plasma cells when antibody synthesis peaks, active *Ig* genes residing on three different chromosomes exhibited pronounced co-localizations in transcription factories, often near the nuclear periphery, displayed trans-chromosomal enhancer interactions, and their transcripts frequently shared inter-chromatin trafficking channels. Conceptually these features of nuclear organization maximize coordinated transcriptional and transcript trafficking control for potentiating the optimal cytoplasmic assembly of resulting translation products into protein multimers.

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

Four publications have resulted this year. One of them reflects a theme from the previous project period, namely the application of fluororous compounds (designer phosphonium salts) in developing electrodes that can detect very small quantities (less than a tenth part per billion) of a troublesome class of persistent environmental contaminants, perfluorosurfactants. Another paper represents an opportunistic catalyst development effort spearheaded by a Chilean exchange student. A novel rhenium-containing phosphine was synthesized and found to be an excellent ligand for palladium catalyzed Suzuki cross-coupling reactions, which see extensive use in the synthesis of pharmaceuticals and agricultural chemicals.

Two publications directly follow from the new directions begun ca. one year ago. One describes the development of metal containing hydrogen bond donors for the polymerization of lactide (available from renewable resources) to polylactide, a biodegradable polymer. Ruthenium and cobalt complexes of 2-guani-dinobenzimidazole, which features five NH linkages, were found to be particularly effective, surpassing the performance characteristics (rates, dispersities, M_n values) of all other hydrogen bond donor catalysts investigated to date (this paper was honored as an "ACS Editors' Choice", a recognition limited to one article per day out of all ACS journals). The other describes a procedure for recycling the Werner trication, $[\text{Co}(\text{en})_3]^{3+}$ and substituted derivatives that is seeing extensive use in work that will be submitted for publication in the near future. For this effort, a scalable synthesis of "fluororous NaBAr_{16} ", a fluorophilic salt of the formula $\text{NaB}(3,5\text{-C}_6\text{H}_3(\text{R}_{16})_2)_4$, was developed. Salts of the type $[\text{Co}(\text{en})_3]^{3+} 3\text{BAr}_6^-$ were then synthesized, and found to readily dissolve in perfluorohexane and similar solvents, which therefore allows them to be easily separated out of complex reaction mixtures and reused. Analogous salts of other polycations similarly partitioned into fluororous phases.

MARGARET E. GLASNER, A-1758, Texas A&M University. WHAT MAKES AN ENZYME PROMISCUOUS? STRUCTURE-FUNCTION RELATIONSHIPS OF *o*-SUCCINYLBENZOATE SYNTHASE/*N*-SUCCINYLAMINO ACID RACEMASE ENZYMES.

This year, we worked on several projects to identify sequence and structural motifs that permit catalytically promiscuous enzymes to use the same active site to catalyze *o*-succinylbenzoate synthesis (OSBS) and *N*-succinylamino acid racemization (NSAR). First, we examined an active site loop in *Amycolatopsis* NSAR/OSBS. One amino acid in the loop makes essential hydrophobic contacts with the substrate and other active site residues. Other residues in this loop form salt bridges with distant amino acids to latch the loop closed. Slight differences in how mutations affect OSBS and NSAR activities suggest that some substitutions in this loop made a small contribution to evolution of NSAR activity, although additional mutations were probably required. This work has been submitted to *Biochemistry*. Second, we began analyzing the roles of other active site residues in *Amycolatopsis* NSAR/OSBS. Mutating an amino acid whose identity differs between promiscuous and non-promiscuous enzymes adversely affected OSBS activity, and proximity to an active site lysine suggested that it could affect the lysine's pK_a. Experiments to determine how it affects both NSAR and OSBS activities at different pH's are underway. We have also identified other positions that could affect specificity for the two activities by analyzing sequence conservation among >500 promiscuous and non-promiscuous NSAR/OSBS enzymes. Finally, we experimentally characterized two other related enzymes to determine the range of their activities. One only catalyzes the OSBS reaction and another is an efficient OSBS but catalyzes NSAR very poorly. We will submit manuscripts on these enzymes in June and in the fall. These enzymes will be the basis for future protein engineering experiments to determine what amino acid changes were necessary and sufficient to achieve efficient OSBS and NSAR activities.

VISHAL M GOHIL, A-1810, Texas A&M University. PHOPHOLIPID-PROTEIN INTERACTIONS IN ENERGY TRANSFORMATION REACTIONS.

One of the three aims of the proposed research plan was to determine the-mechanism by which meclizine, an over-the-counter anti-nausea drug, inhibits mitochondrial respiration. Based on our initial finding that meclizine directly inhibits a phospholipid biosynthetic enzyme, phosphoethanolamine cytidyltransferase (Pcyt2), we had hypothesized that meclizine inhibits mitochondrial respiration either by: (1) accumulation of phosphoethanolamine (PEtn), a Pcyt2 substrate or (2) diminution of phosphatidylethanolamine (PE), a downstream product of Pcyt2. We tested these two possibilities and showed that:

- 1) PEtn inhibited ADP-stimulated mitochondrial respiration with an IC₅₀ of approximately 3 mM. The inhibition was observed in isolated suspension of mitochondria, suggesting that PEtn directly targets mitochondria.
- 2) The intracellular concentration of PEtn following five hours of meclizine treatment increases to 4 mM, a concentration sufficient to inhibit mitochondrial respiration.
- 3) The cellular and mitochondrial PE levels following meclizine treatment are not significantly affected, suggesting that meclizine effect is likely mediated through accumulation of PEtn and not depletion of PE.
- 4) PEtn reduced mitochondrial membrane potential and decreased NADH and FADH₂ levels, suggesting that it inhibits mitochondrial respiration by interfering with the generation of reducing equivalents. This mechanism of respiratory inhibition appears to be distinct from any of the previously known agents.

Taken together, these results elucidated a novel mechanism by which meclizine inhibits respiration. Our results are significant not only in terms of discovering novel biochemical activity of a clinically used drug but it also sheds new insights on the regulation of respiration by a non-mitochondrial phospholipid pathway.

IDO GOLDING, Q-1758, Baylor College of Medicine. QUANTIFYING TRANSCRIPTION KINETICS IN INDIVIDUAL CELLS AT SINGLE-EVENT RESOLUTION.

(i) *Detect active transcription in individual E. coli cells.* Going beyond the measurement of total mRNA copy number from a gene of interest in the cell, we have developed different approaches to distinguish nascent mRNAs (i.e. now being actively produced) from mature mRNAs that are diffusing in the cytoplasm. Telling those two populations apart will allow us to quantify the activity of the gene at a much finer temporal resolution. (ii) *Quantify stochastic regulation by transcription factors in the early Drosophila embryo.* We simultaneously labeled, and quantified, the transcription factor Bicoid and nascent mRNA produced from the gene it regulates, *hunchback*, in individual nuclei of the embryo. Analyzing the complete single-nucleus data set allowed us to elucidate which parameters of stochastic gene activity are modulated by the transcription factor. Furthermore, we were able to simultaneously quantify the binding of transcription factor at the promoter and relate this binding to the observed gene activity. (ii) *Extract the parameters of stochastic transcription kinetics in mouse embryonic stem cells.* We measured the copy numbers of both nascent and mature mRNAs for a number of key genes in individual mouse embryonic stem cells. The data set was then used, in conjunction with a theoretical model, to evaluate the kinetic parameters characterizing the stochastic transcription kinetics of each gene.

ELIZABETH J. GOLDSMITH, I-1128, The University of Texas Southwestern Medical Center. DOCKING INTERACTIONS BETWEEN THE MAP3Ks, ASK1/TAO2 AND B-Raf WITH THEIR COGNATE MAP2Ks MEK6 AND MEK1.

In the past year, we have continued our studies of the phosphorylation of p38 MAP kinase by MEK6, and the phosphorylation of MEK6 by TAO2 and the paper has been published. We further wrote a review paper on this work that has been submitted. We engaged in progress-curve differential equation modeling to determine which of the elemental kinetic steps in the activation of MAP kinase modules actually contributes to the kinetic outcome. This is

described in the paper. The results reveal significant persistence of protein-protein interactions, suggestive that switch-like behavior of the cascade observed in cells can possibly arise from these phosphorylation events alone, without any other factors required, such as feedback.

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

Electronic properties: One paper is an invited perspective on the engineering of transition-metal oxides. Tailoring the redox energies of transition-metal oxides is important for the electrodes and electrolyte of electrochemical devices. Papers were submitted that investigated electrode materials for rechargeable Na-ion batteries; papers submitted also explored electrode and electrolyte materials for Li-ion batteries. One article was part of a collaborative work on oxide catalyst for air electrodes of batteries and room-temperature fuel cells.

In another paper, a study of the magnetic properties of the $A_{1-x}A_x\text{RuO}_3$ perovskites ($A, A' =$ alkaline earth) has clarified the evolution of ferromagnetism on traversing the crossover from itinerant to localized electron behavior on the RuO_3 sublattice. One published article demonstrates that under high pressure, the perovskite PbRuO_3 forms an unprecedented Pb-Ru bond. Another publication shows the influence of A-site Cu on the spin-spin interactions between B-site Fe in the double perovskite $(\text{CaCu}_3)\text{Fe}_2\text{Sb}_2\text{O}_{12}$. Another article investigates the electronic properties of BaIrO_3 where the spin-orbit coupling of the $5d$ electrons is strong. Another article reports the role of an internal electric field in layered NaLiTiO_3 on the ferric Ti displacements and another paper the pressure dependence of the superconductive transition temperature in $\text{YFe}_4\text{P}_{12}$.

Oxide-ion electrolytes. We have identified two oxide-ion electrolytes permitting a solid oxide fuel cell operating below 500°C that will be studied for H_2 production from steam and in a novel medium-temperature rechargeable battery.

DAVID G. GORENSTEIN, AU-1296, The University of Texas Health Science Center at Houston. COMBINATORIAL SELECTION, STRUCTURE AND DESIGN OF NEXT GENERATION X-APTAMERS.

A bead-based DNA X-aptamer combinatorial library was synthesized with permonothioated backbones and allylamino substitutions (1,048,576 sequences). The bead-based library was screened with CD44 and the best binding sequences were identified after PCR, sub-cloning. By combining our random bead-based aptamer library development methods with conjugation chemistry techniques, we have created a next-generation of aptamers, X-aptamers (XAs). Several different duo ligands (such as ADDA and other small molecules in red and green, see above Figure; structure based upon ^{15}N - ^1H HSQC 2D NMR spectral changes of CD44 upon binding X-aptamer) can be added in a directed or random fashion to the aptamers to further enhance their binding affinity to the target protein. We have succeeded in identifying the first example of an X-aptamer and to increase the binding of the small molecule to the protein by over 1,000,000-fold. We now are trying to develop the X-aptamer as a scaffold to fold and present two different small molecules covalently attached to the oligo. Preliminary data indicates enhanced binding as well.



KAYLA N. GREEN, P-1760, Texas Christian University. PROBING SURFACE INTERACTIONS OF FERROCENE PEPTIDE CONJUGATES AND INTERFACIAL RESPONSES WITH BIOMOLECULES.

Overall, we have reported the synthetic methods (Figure 1) to produce ferrocene bioconjugates that can be immobilized on a gold surface. As ferrocene-bioconjugates similar to **1** have applications as potential biosensors, overcoming these synthetic difficulties is paramount. Using solid-phase methods akin to solid-phase peptide synthesis, we have produced a well characterized bioconjugate **1** that contains biotin-ferrocene-cysteine. Furthermore, we have shown through SEM that this system is able to adhere to a gold surface thanks to the thiolate moiety of the cysteine component.

We have also carried out molecular modeling using AutoDock Vina to show that the ferrocene component of Bioconjugate **1** does not interfere with the biotin-avidin interaction (Figure 2). The resulting models showed interactions of **1** in the expected binding sites of avidin but only random interactions were observed between **1** with albumin. The latter interaction appeared to be driven by weak intermolecular forces.

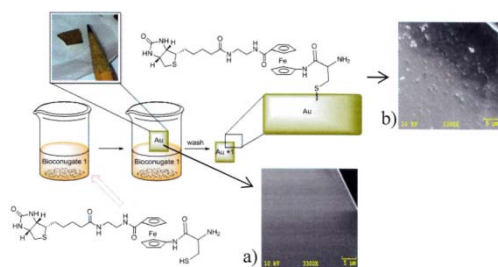


Figure 1. Schematic drawing representing the immobilization of **1** onto a gold slide. The top inset is a photograph showing the size of a representative gold slide in comparison to a pencil. SEM images of gold layered onto a plastic-polymer film are shown after (a) incubation sans **1** and (b) following incubation with **1** in water overnight and rinsing with water.

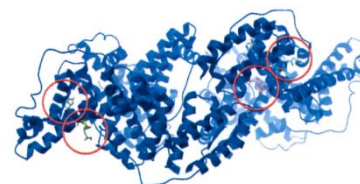


Figure 2. Overlay of the 4 lowest energy models derived from **1** + Avidin using AutoDock Vina. **1** is circled in red.

PAOLO GRIGOLINI, B-1577, University of North Texas. ERGODICITY BREAKING IN CHEMICAL, BIOLOGICAL AND COOPERATIVE SYSTEMS.

In the case of sub-diffusion we have proposed a new model where both trapping and memory are present. We simulated the trapping process by using a fractional rather than ordinary derivative in time and the infinitely extended memory by replacing the conventional time independent diffusion coefficient with a power law function of time. We have also explored the cooperative origin of the fractional derivative in time and the effect of environmental noise on the correlated dynamics of many cooperating units. These papers establish a surprising connection between anomalous diffusion in living cells and neurophysiological systems at criticality.

In spite of the apparent simple structure of the diffusion equation describing the joint action of trapping and memory of, this equation yields an algorithmic challenge that we have successfully addressed. The discussion of the cooperative origin of dynamics described by means of fractional calculus led to the discovery that the transmission of information from a complex to another complex network is realized through the extended process of transition to equilibrium, in spite of the ordinary statistical physics emerging in the large time limit.

Finally, we have adopted the first-passage time observation to establish the contribution of trapping and memory to biological sub-diffusion.

NICK V. GRISHIN, I-1505, The University of Texas Southwestern Medical Center. STRUCTURE MECHANISM OF CIRCADIAN CLOCK-MEDIATED TRANSCRIPTION ACTIVATION.

We have generated a number of constructs of CLOCK:BMAL1, including the heterodimer of bHLH-PASAB domains of CLOCK and BMAL1, the Exon 19 domain of CLOCK, and a C-terminal helical region of BMAL1. These domains have been purified to homogeneity. A series of overlapping constructs of p300/CBP fragments have also been made and we are currently working on purifying sufficiently large quantities of these protein domains for protein-protein interaction screens. Several assays such as pull-down, size-exclusive chromatography, and isothermal titration calorimetry (ITC) are planned.

Additionally, we have performed a bioinformatics analysis of various mammalian clock proteins and a number of coactivators and repressors that were reported to interact with CLOCK:BMAL1, including p300/CBP, histone methyltransferase MLL1, and a repressor CIPC. Based on this analysis, we propose that the Exon 19 domain of CLOCK is likely to adopt a coiled-coil helical conformation. Interestingly, a coiled-coil helical region is also identified in the C-terminal region of CIPC and within residues 354-450 of MLL1, but not in any other clock proteins and coactivators that we studied. Both CIPC and MLL1 were reported to interact with CLOCK Exon 19. While we have co-expressed and copurified CLOCK Exon19 and CIPC, we are now starting to investigate the potential interaction between CLOCK Exon 19 and the coiled-coil domain of MLL1. Results obtained from these studies should provide new insights into the clock-mediated transcription activation mechanism.

ARNOLD M. GULOY, E-1297, University of Houston. CHEMICAL BONDING AND PROPERTIES OF "ELECTRON-POOR" INTERMETALLICS ALONG THE ZINTL BORDER.

We continued our investigations on the chemistry of complex polar intermetallic compounds - electron-poor main group Zintl phases (inorganic intermetallics) and transition metal Zintl phases; metal-rich subcompounds (suboxides, subhalides and subnitrides); and complex metal chalcogenides. Exploratory synthetic studies, coupled with detailed structural and physico-chemical characterization were performed. Subsequent studies on their reactivity (mild redox) and solution chemistry were also initiated. In particular, exploratory syntheses via mild oxidation reactions of Zintl phases and low dimensional polar intermetallics in polar solvents and ionic liquids are in progress. The highlight of this year's accomplishments is the discovery and subsequent characterization of a novel layered titanium-based pnictide superconductor, $Ba_{1-x}NaTi_2Sb_2O$ ($x = 0-33$). The novel compound was found to exhibit both magnetic ordering (spin density wave (SDW)) and superconductivity, akin to the high-Tc cuprates and FeAs-based superconductors, albeit with lower Tc's. A full characterization of the material, including transport, magnetic, vibrational spectroscopy, and electronic structure calculations, as well as the nature of the superconductivity were reported and reviewed. A further search for related layered intermetallic and related metal-rich compounds are currently in progress.

Studies on related low-dimensional layered chalcogenides have also led to a unique and effective single crystal growth technique for layered metal chalcogenides. A useful chemical exfoliation route was developed to provide unique samples of single-layer and ultrathin layers of metal chalcogenides with enhanced properties for molecule-based devices and field effect nano-transistors. The technique is being extended to other layered materials - germanides, silicides and pnictides.

JASON H. HAFNER, C-1761, Rice University. ANALYTICAL SURFACE ENHANCED RAMAN SPECTROSCOPY FOR BIOLOGICAL INTERFACES.

We published some chemical insights into the synthesis and properties of gold nanobelts, but have concluded that they are not useful SERS substrates for this project due to their non-uniform structure at the nanometer scale. We have therefore focused our effort entirely on the more successful gold nanorods with membrane coatings in solution. Using our high-sensitivity spectrometer built last year, we have confirmed that the lipid coating is indeed a fluid bilayer with properties similar to natural membranes. The individual intensities of seven specific SERS bands of phosphatidylcholine were identified with help from density functional theory calculations of the Raman tensor using a commercial package (Amsterdam DFT). Their relative intensities indicate lipids arranged normal to the nanorod surface. We measured lipid exchange between the nanorod surface and vesicles in solution using deuterated lipids, which confirms a fluid bilayer with only weak interaction with the gold surface. Finally, we detected the fluid/gel phase transition by tracking the nanorod optical properties as a function of temperature. This very sensitivity transition temperature exactly matched that of free lipid bilayer vesicles in solution. A comprehensive article on these results will be submitted in the coming weeks.

NAOMI J. HALAS, C-1220, Rice University. CHEMICAL AND PHOTOPHYSICAL PROPERTIES ON COMPLEX NANOPARTICLES AND NANOPARTICLE COMPLEXES.

Highlights from our previous year's research includes investigating the optical properties of well defines 3D clusters of nanoparticles (NPs); fluorescence enhancement of dyes; synthesis of sub 100 nm hollow gold nanoshells (HGNS) of three different sizes, while maintaining the same NW resonance; alternate plasmonic materials; and identification of single analyte molecule using surface enhanced coherent antistokes Raman scattering (SECARS).

We investigated the optical properties of well defined stable nanoparticle clusters (2-19 NPs) whose optical properties are either highly sensitive or remarkably independent of orientation. We demonstrated fluorescence enhancement from three different dye molecules embedded in the interstitial SiO₂ layer of Nanomatryoshka NPs that exhibit Fano resonances. We synthesized sub 100 nm HGNS of three different sizes through a galvanic replacement of a sacrificial Ag core. A theoretical model indicated that alloying, residual Ag in the core and NP porosity contributed to the constant NIR resonance. We are investigating Aluminum as an isotopically abundant and less expensive alternate material to Au and Ag for plasmonic applications and for extending plasmonics into the UV region. Hot electron induced photo dissociation of H₂ on Au NPs on a SiO₂ substrate was investigated and shows two orders of magnitude increase as compared to similar gold NPs on a TiO₂ substrate. We have demonstrated, for the first time, single molecule detection sensitivity, using Fano resonant NP clusters to enhance the SECARS signal from molecules with a small Raman cross section.

P. SHIV HALASYAMANI, E-1457, University of Houston. ADVANCED SECOND-HARMONIC GENERATING MATERIALS.

We have synthesized and characterized several new oxide compounds that exhibit second-harmonic generation (SHG), as well as other functional properties such as ferromagnetism and pyroelectricity. Our strategy, to use cations susceptible to second-order Jahn-Teller effects, i.e, octahedrally coordinated d⁰ transition metals (Ti⁴⁺, Nb⁵⁺, W⁶⁺, etc.) and cations with a lone-pair (Se⁴, Te⁴⁺, I⁵⁺, etc.) has substantially increased the incidence of acentricity in any new material. In using this design strategy we have synthesized a variety of new non-centrosymmetric materials including Na₂(WO₃)₃(SeO₃)₂·2H₂O, Na₆(W₆O₁₉)(SeO₃)₂ and Li₂VPO₆. In addition, we have collaborated on the investigation of new magnetically ordered polar materials - Mn₂FeMO₆ (M = Nb, Ta) and Ba₂YFeO_{5.5}. Finally, we published a chapter on the chemistry of polar transition metal oxides in Comprehensive Inorganic Chemistry II - the update to Comprehensive Inorganic Chemistry I published in 1973. We are continuing to expand our synthetic efforts, as well as develop structure-property relationships and single crystal growth.

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

Density functional theory (DFT) calculations on the reactions and electronic structure of heavier group 14 elements formed a major component of this year's contributions.

DFT calculations with the polarizable continuum model (PCM) for solvation has been used to study the mechanism of the addition of trans-(2-phenylcyclopropyl) -carboxaldehyde to dimesitylfluorenylidene-germane. Two different pathways have been observed in the experiment, including [2 + 2] addition and [4 + 2] addition. The reaction is strongly influenced by the choice of solvent: the [4 + 2] addition product, 1,2-oxagermin, was the major product in benzene, while the [2+2] addition product, tetramesityl-1,3-dioxadigermetane and fluorenylidene-(trans-2-phenylcyclopropyl)methane were the major products in THE The computations reveal that the different mechanisms are favored in the polar vs. non-polar solvent because the [2 + 2] pathway generates a more polar transition state.

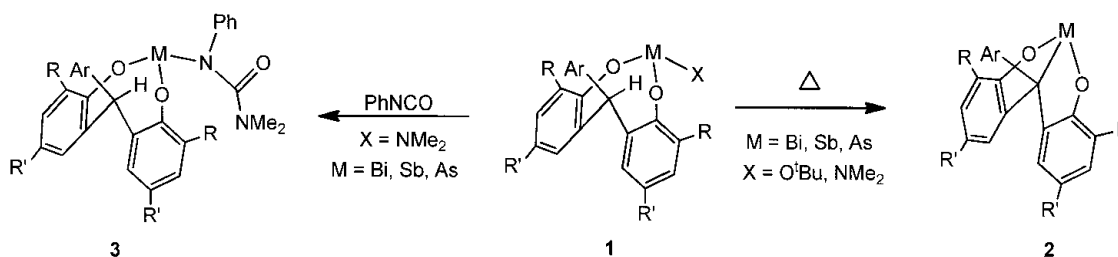
DFT computations on [Cp*(ⁱPr₃P)(H)Os≡Si(Trip)][HB(C₆F₅)₃] support the presence of a silylyne ligand, the first ever reported for osmium. NBO and ETS-NOCV analysis revealed the nature of this Os-Si interaction as a triple bond consisting of a covalent σ bond and two strong π back-donations. The Os≡Si adds terminal alkynes *via* C-H bond addition, while diphenylacetylene adds the C-C bond across the Os≡Si bond.

TRACY A. HANNA, P-1737, Texas Christian University. INTRAMOLECULAR BISMUTH AND ANTIMONY-CARBON BOND FORMATION AND REACTIVITY.

Graduate student Alane Nunez and postdoctoral associate Sitaram Acharya have completed their study of heavy Group 15 element bisphenolates, 1. They have characterized examples of bisphenolates for M = Bi, Sb, and As, and R = O^tBu and NMe₂. Ms. Nuñez's reactivity studies have included investigation of C-H activation of the bisphenol methylene linker to form complexes 2, as well as insertion reactions into the M-N bond (when R = NMe₂), exemplified by product 3.

In her insertion chemistry studies, Ms. Nuñez has also investigated reactivity of complex 1 with metal halides, heterocumulenes, AlMe₃, Me₃SiCl, and a range of acids, but was unable to crystallographically confirm her proposed products. Ms. Nuñez defended her dissertation in July, and expects to graduate in December 2013.

Postdoctoral associate Dr. Sitaram Acharya also combined his expertise in low-valent molybdenum catalysis with our focus on calixarene and bisphenolate chemistry. He prepared low-valent molybdenum calixarene and bisphenolate complexes and investigated the catalytic reactivity of these, as well as his metal carbonyl and metal phosphine synthons, in the epoxidation of alkenes. He is currently preparing a manuscript describing this work. The chapter titled "Coordination chemistry and applications of phenolic calixarene-metal complexes" was completed and is under publication as part of the Patai series book *Metal Phenolates*.



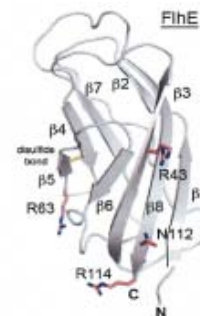
JOHN C. HARDY, A-1397, Texas A&M University. NUCLEAR DECAY STUDIES.

In 2012-13 we reached our goal to develop a data-acquisition system capable of measuring branching ratios for short-lived ($t_{1/2} < 1$ s) superallowed beta-transitions to a precision of 0.1% in the presence of other strong branches. This past year, 2013-14, we finished and published a measurement of the decay of ³⁸Ca, our first experiment with this world-leading system. The result completes the full characterization of a mirror pair of superallowed transitions - ³⁸Ca → ³⁸K^m and ³⁸K^m → ³⁸Ar - and constitutes the first step in our plan to constrain the calculated isospin-symmetry-breaking corrections that must be applied to all superallowed data. We have already taken branching-ratio data on a second such superallowed case, the decay of ³⁴Ar; had preliminary tests of two more, ³⁰S and ⁴²Ti; and have scheduled cyclotron beam time in August to measure a fourth, ²⁶Si. Together, these measurements will ultimately lead to higher precision both in our extracted value for the weak vector coupling constant and in the universality test of the weak force. In parallel, we are also seeking to further improve our precision in the measurement of half-lives. To this end, we are currently comparing our standard analog system with two new digital systems we have developed to see if the latter offer promising opportunities. In the second component of our program, we have published our precise measurement of the K-shell internal conversion coefficient (ICC) for an M4 transition in ¹¹⁹Sn; have completed a new measurement on ¹²⁷Te; and will measure another, ¹¹¹Cd, this summer. These measurements are widening the range and depth of our tests of calculated internal conversion coefficients.

RASKIA M. HARSHEY, F-1811, The University of Texas at Austin. STRUCTURAL CHARACTERIZATION OF A NOVEL REGULATOR OF H⁺ FLOW ACROSS THE BACTERIAL MEMBRANE: A POTENTIAL ANTI-MICROBIAL DRUG TARGET.

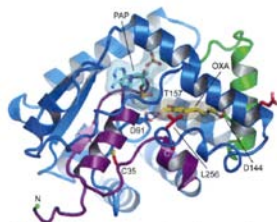
We have completed the first aim of the proposal by solving the structure of FlhE. This is reported pictorially below.

FlhE structure and sequence alignment. The β-sandwich fold of the protein, a 114 residue monomer, is unique in the Protein Data Base. Amino acid alignment of FlhE from *Salmonella enterica* with the FlhE's from 33 other flagellated bacteria shows which residues are conserved (arrows indicate >90% identity). Through a comparison with the structure, highly conserved surface residues can be identified. Side chains of R43, R63, N112 do not play a structural role, and hence are likely to serve a functional role. These residues will be subjected to mutagenesis for functional studies.



P. JOHN HART, AQ-1399, The University of Texas Health Science Center at San Antonio. STRUCTURE AND ACTION OF A *SCHISTOSOMA MANSONI* SULFOTRANSFERASE IMPLICATED IN DRUG RESISTANCE.

During the first year of the award, we expressed, crystallized and determined the 1.7 Å structure of the *S. mansoni* sulfotransferase (SmSULT) in complex with 3'-phosphoadenosine-5'-phosphate (PAP), the depleted form of the co-factor for these enzymes, PAPS (3'-phosphoadenosine-5-phosphosulfate). We also determined the structure of SmSULT•PAP in complex with oxamniquine (OXA) (see Figure at right). Together the structures reveal the molecular basis for OXA action against *S. mansoni*. These data were published in *Science* in late 2013 [Valentim et al. *Science* 342, 1385-1389]. Although the *S. mansoni* enzyme (SmSULT) is ~70% identical to the *S. haematobium* ortholog (ShSULT) and ~52% identical to the *S. japonicum* ortholog (SjSULT), OXA fails to kill the latter two species. We have initiated efforts to determine the structures of the ShSULT and SjSULT enzymes for comparative analyses and ShSULT crystals are now in-hand. The ShSULT and SjSULT structures will guide the design of OXA-like analogs that are effective killing agents against *S. haematobium* and *S. japonicum*.



Schistosoma mansoni sulfotransferase (SmSULT, ribbons) with bound 3'-phosphoadenosine-5'-phosphate (PAP, cyan sticks) and oxamniquine (OXA, yellow sticks). Taken from Valentim et al. (2013) *Science* 342, 1385-1389.

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

This funding year has resulted in three publications. The first, published in *Biomacromolecules*, describe our advances with β -sheet nanofiber hydrogels. In this work we show how the unique self-assembling nature of these hydrogels can be used to encapsulate stem cells. Six different peptide sequences were compared for their ability to promote cell proliferation, adhesion and spreading. The second, published in *J. Am. Chem. Soc.*, describes the design and characterization of a non-canonical collagen triple helix. We show how carefully designed charge pairs can control triple helix assembly into sticky-ended helices offset by four amino acids instead of the normal single amino acid offset. The third paper, also published in *Biomacromolecules*, describes the use of our designed collagen hydrogels as a medical material. In particular we show that our synthetic, self-assembled collagen hydrogels are able to clot blood in a rapid fashion. This material has the potential to replace naturally sourced collagen (usually from animals) which would have the advantage of having fewer contamination, immune response and inflammatory problems.

ADAM HELLER, F-1131, The University of Texas at Austin. DESIGN OF POLYMERIC BINDER-CARBON PARTICLE COMPOSITES OF LITHIUM ION BATTERY ELECTRODE.

The Welch Foundation supported our design and synthesis of enzyme-wiring redox polymers between 1989 and 2005; the University of Texas licensed the technology to TheraSense, acquired by Abbott Laboratories in 2004, now the major part of Abbott Diabetes Care. In August 2014 (in Europe) and early 2015 (in the US) Abbott Diabetes Care (ADC) will introduce a miniature, bloodless, accurate, wired-enzyme based, continuously glucose monitoring system, intended to replace the 10 billion single-use strips used annually for blood glucose monitoring. Its core subcutaneously implanted sensor is easily and painlessly self-replaced by the user every 14 days. Although the thicknesses and other properties of the sub-dermis receiving the implant differ between users, the same factory-pre-calibrated sensor is used in all. The user reads his or her glucose concentration by swiping a mobile phone-like reader over the implanted skin, obtaining both the current concentration, as well as historical data for the previous eight hours. A type I diabetic user would use about 70 strips and a type 2 diabetic user would use about 20 strips in a 14 day period.

The simplest electro-osmotic pump, consisting merely of a ceramic frit sandwiched between two plasma oxidized carbon cloth electrodes, has been built and tested. (*ChemElectroChem* 1, 868-870 (2014).

Ge and Sn-Cu, two high rate sodium anodes for sodium ion batteries were reported in both the *Journal of Physical Chemistry C* 117(37), 18885-18890 (2013) and *ACS Applied Materials & Interfaces* 5(17), 8273-8277 (2013). PbTe and slurry-cast Ge, both high rate lithium ion battery anode materials were reported. (*Journal of Materials Chemistry A: Materials for Energy and Sustainability* 2(20), 7238-7243 (2014); *Journal of Power Sources* 238, 123-136 (2013).

RYAN E. HIBBS, I-1812, The University of Texas Southwestern Medical Center. STRUCTURAL BASIS OF CHEMICAL TRANSMITTER RECOGNITION BY PENTAMERIC LIGAND-GATED ION CHANNELS.

The progress in the past year, the first year of this grant, involved (1) optimizing an $\alpha 7$ receptor construct for large scale expression and crystallization, and (2) setting up the first crystallization trials. Toward the first goal, we screened approximately one hundred constructs and optimized expression conditions to the point that we now can produce ~1 mg protein from 1 L of cells, by baculovirus transduction and affinity and gel filtration chromatography. This protein preparation is stable for >1 week at 4 °C. Attempts at crystallizing this purified receptor alone have thus far been unsuccessful, so we are pursuing two alternative pathways. First, we raised monoclonal antibodies against the receptor for the purposes of co-crystallizing the receptor bound to Fab fragments. We were excited to identify several antibodies that bound to the $\alpha 7$ receptor in a conformation-dependent manner. Specifically, we found antibodies that selectively recognized open-activated, closed-resting and desensitized receptor states. We have now isolated Fab fragments from these antibodies and co-purified the $\alpha 7$ receptor-Fab complexes. Crystallization experiments are underway. The second, parallel strategy involves cryo-EM of the same samples we are now using also for crystallization. We have preliminary, very promising images of $\alpha 7$ -Fab complexes where we can easily visualize the subunits of the receptor forming the pore as well as five Fab molecules binding to the receptor like blades on a propeller.

PETER R. HIESINGER, I-1657, The University of Texas Southwestern Medical Center. THE ROLE OF THE V0 ATPASE IN SNARE-MEDIATED MEMBRANE FUSION.

In April 2014 we have published our findings on Calcium/Calmodulin regulation of SNARE assembly through V100. Chemical neurotransmission occurs through Ca^{2+} -dependent evoked or spontaneous vesicle exocytosis. In both cases, Ca^{2+} sensing is thought to occur shortly before exocytosis. We now showed that the Ca^{2+} -dependence of spontaneous vesicle release may partly result from an earlier requirement of Ca^{2+} for the assembly of soluble N-ethylmaleimide-sensitive fusion attachment protein receptor (SNARE) complexes. We further showed that the neuronal v-ATPase V0 subunit a1 (V100) can regulate the formation of SNARE complexes in a Ca^{2+} /Calmodulin-dependent manner. Ca^{2+} /Calmodulin regulation of V100 is not required for vesicle acidification. Specific disruption of the Ca^{2+} -dependent regulation of V100 by Calmodulin led to a >90% loss of spontaneous release, but only had a mild effect on evoked release at *Drosophila* embryo neuromuscular junctions. Our data suggest that Ca^{2+} /Calmodulin regulation of V100 may control SNARE complex assembly for a subset of synaptic vesicles that sustain spontaneous release. Publication of SNARE-binding-deficient V100 is planned for 2014.

CHRISTIAN B. HILTY, A-1658, Texas A&M University. STRUCTURE AND FOLDING OF MEMBRANE TARGETED PEPTIDES.

Two membrane associating peptides, the antimicrobial peptide Magainin2 from *X. laevis*, and a G1V mutant of the hemagglutinin (HA) fusion peptide from the influenza virus, were characterized by circular dichroism (CD) spectroscopy and NMR. Thermally induced unfolding was measured in detergent micelles of different charge (anionic sodium dodecyl sulfate [SIDS], zwitterionic dodecyl phosphocholine [DPC] and cationic dodecyl trimethylammonium chloride [DTAC]). Magainin2 has an overall charge of +3, while HA G1V has a net charge of -3 at neutral pH. The temperature dependence of CD signal at 222 nm for magainin2 showed greatest curvature in DTAC, but for HA G1V showed greatest curvature in SIDS. In each case, greatest curvature was observed in the presence of like charge and least curvature in the presence of unlike charge on the peptide and the micelle. This result suggests an increased cooperativity in the helix-coil transition of the peptide in the presence of like charges. The cooperativity may be mediated by the effect of electrostatic interactions. Residue specific effects of electrostatic interactions were further investigated by measuring the temperature dependence of chemical shifts and Nuclear Overhauser effect (NOE) cross-peak intensities of magainin2 in SIDS and DPC detergent micelles. While Chemical shift temperature coefficients in the two micelles were comparable, the temperature dependence of NOEs diagnostic for alpha-helical secondary structure showed a greater difference between the hydrophobic and the hydrophilic face of the peptide in DPC compared to SIDS. This suggests that the presence of negative charges on the SIDS micelles may add to the stability of the hydrophilic face of the cationic peptide.

DAVID M. HOFFMAN, E-1206, University of Houston. SYNTHESIS OF METAL COMPLEXES WITH STERICALLY ENCUMBERED KETIMIDE LIGANDS.

Ketimide ligands, $\text{RR}'\text{C}=\text{N}^-$, are single-faced π donor and acceptor ligands in which the π donor and acceptor orbitals are orthogonal. Earlier, we reported that this π donor-acceptor capability led to the unusual diamagnetism of $d^2 D_{2d}$ $\text{Cr}(\text{N}=\text{C}-t\text{-Bu})_4$. In an attempt to synthesize lower coordination-number complexes, $\text{LiN}=\text{C}-t\text{-Bu}_2$ was allowed to react with CrCl_2 . This produced the diamagnetic Cr(II) dimer $[\text{Cr}(\mu\text{-N}=\text{C}-t\text{-Bu}_2)(\text{N}=\text{C}-t\text{-Bu}_2)]_2$, which a single-crystal X-ray structure revealed has a "butterfly" structure with three-coordinate Cr(II) centers and a short Cr-Cr bond length (2.08 Å). In contrast, the few other reported Cr(II) complexes of the type $[\text{Cr}(\mu\text{-X})_2]$ where X = amide or alkoxide all have long Cr-Cr bond lengths (>2.85 Å). A bonding analysis suggests $[\text{Cr}(\mu\text{-N}=\text{C}-t\text{-Bu}_2)(\text{N}=\text{C}-t\text{-Bu}_2)]_2$ has a $\sigma^2\pi^4\delta^2$ quadruple bond. The reaction of CoCl_2 with three equiv of $\text{LiN}=\text{C}(\text{C}_6\text{H}_2-2,4,6-i\text{-Pr}_3)_2$, followed by oxidation with I_2 , yielded Co(III) $\text{Co}(\text{N}=\text{C}(\text{C}_6\text{H}_2-2,4,6-i\text{-Pr}_3)_2)_3$. A single-crystal X-ray analysis revealed a three-coordinate trigonal-planar structure akin to the previously reported Co(III) complex $\text{Co}(\text{N}(\text{SiMe}_3)_2)_3$. A similar reaction by using $\text{LiN}=\text{C}-t\text{-Bu}(\text{C}_6\text{H}_2-2,4,6-i\text{-Pr}_3)$ and CoCl_2 yielded unexpectedly the Co(II) dimer $[\text{Co}(\mu\text{-N}=\text{C}-t\text{-Bu}(\text{C}_6\text{H}_2-2,4,6-i\text{-Pr}_3))(\text{N}=\text{CC}_6\text{H}_2-2,4,6-i\text{-Pr}_3)]_2$, where the terminally bonded nitrile $\text{N}=\text{CC}_6\text{H}_2-2,4,6-i\text{-Pr}_3$ resulted from the loss of a ketimide *t*-Bu substituent. Magnetic studies on Co(III) $\text{Co}(\text{N}=\text{C}(\text{C}_6\text{H}_2-2,4,6-i\text{-Pr}_3)_2)_3$ and Co(II) $[\text{Co}(\mu\text{-N}=\text{C}-t\text{-Bu}(\text{C}_6\text{H}_2-2,4,6-i\text{-Pr}_3))(\text{N}=\text{CC}_6\text{H}_2-2,4,6-i\text{-Pr}_3)]_2$ are in progress. In collaborative work, SnO_2 thin films containing SnO_2 -coated gold nanoparticles were prepared by sol-gel for optoelectronic applications, and gold shell/silica core particles were synthesized and incorporated into organic polymeric thin films for thermal energy collection applications.

BRADLEY J. HOLLIDAY, F-1631, The University of Texas at Austin. SEEDED GROWTH OF INORGANIC MATERIALS WITHIN ORGANIC TEMPLATES.

To date, efforts toward achieving solar energy conversion, including photocatalysis, have been hampered by high-cost and low overall efficiency. We believe that the solution to this scientific problem will only be found by the development of fundamentally new materials. In sharp contrast to conventional systems based on physical mixtures of organic polymers and inorganic semiconductors or metallic materials, our chemical methodology is based on a controlled seeded-growth approach within conducting metallopolymer materials. In this grant year, we have made progress in three main areas. First, the systematic synthesis and detailed study of fundamentally new conducting metallopolymers has been accomplished. With these materials, we have shown that the metal centers incorporated into well-known conducting polymer systems can have profound impacts on the level and mechanism of electrical conductivity. Second, the preparation of a series of rhenium-containing conducting metallopolymers has allowed us to explore the electrocatalytic activity of this class of materials. These are important materials to develop because the direct transformation of environmentally damaging carbon dioxide directly into useful chemical feedstocks can be achieved with these types of electrocatalysts. Third, we have been recently exploring the incorporation of a new type of organic semiconducting unit, thieno[3,2-b]thiophene, into conducting metallopolymer materials. These studies have important implications for the design of optoelectronic, electrocatalytic, and photocatalytic materials that will have increased lifetimes as we have demonstrated that these moieties are more chemically robust under light irradiation than traditional semiconducting polymer segments.

LORA V. HOOPER, I-1762, The University of Texas Southwestern Medical Center. BIOCHEMICAL AND STRUCTURAL STUDIES OF A NOVEL RETINOID BINDING PROTEIN FAMILY.

During the past year we have substantially advanced our understanding of how SAAs bind to retinoids. Our major breakthrough was in determining the crystal structure of mouse SAA3 (mSAA3). The protein was crystallized in a $P6_2$ space group with two subunits in the asymmetric unit, and the structure was determined to a resolution of 2 Å by single-wavelength anomalous dispersion (SAD) phasing using a selenomethionyl-derivatized crystal. The crystal structure revealed that mSAA3 is highly α -helical and forms a tetramer with a hydrophobic interior that is protected from the external aqueous environment. The tetrameric structure is supported by size exclusion chromatography and cross-linking experiments that show that mSAA3 forms a tetramer in solution. We were unable to obtain mSAA3 crystals with the bound retinol ligand as retinol is highly unstable and the crystals required several weeks to grow. However, a ligand docking analysis using SwissDock indicated that retinol can be docked in this hydrophobic pocket with favorable free energy (~ -7 kcal/mol) and FullFitness values (~ 2400 kcal/mol). Consistent with this prediction, introducing a Trp71Ala (W71A) mutation in the mSAA3 hydrophobic core reduced the affinity of mSAA3 for retinol. Thus, the mSAA3 structure supports our biochemical data showing a retinol binding function for SAAs and explains how mSAA3 could bind retinol. Altogether, our results from this study identify SAAs as a family of microbe-inducible retinol binding proteins, reveal a unique protein architecture involved in retinol binding, and suggest how retinol is circulated during infection

JENNY HSIEH, I-1660, The University of Texas Southwestern Medical Center. CHEMICAL REGULATION OF ADULT HIPPOCAMPAL NEUROGENESIS.

This past year, we obtained Fmr1 KO and WT mice from Dr. Kimberly Huber (Dept. Neuroscience, UTSW) and have performed the following:

1. Expanded breeding of Fmr1 WT and KO mice for adult neurogenesis studies.
2. Treated Fmr1 WT and KO mice with 7 days of *Isx-9* or vehicle control (IP) in two sets of experiments as detailed in our proposal. In Exp 1, we killed the mice after 7 days of *Isx-9* treatment and performed BrdU labeling (one injection two hours before sacrifice) to determine changes in neural stem cell proliferation. In Exp 2, we killed the mice after 4 weeks (BrdU was injected for the first week) to determine changes in new newborn neuron survival.
3. We are currently performing immunostaining of BrdU, markers of new neurons/dendrites and fluorescence microscopy to quantify changes in adult neurogenesis. Our plan for next year is to finish the histology experiments. If we detect changes between WT and Fmr1 KO mice treated with *Isx-9*, we will breed the mice for behavior testing.

HUEY W. HUANG, C-0991, Rice University. THE FREE ENERGY PATHWAY FOR LIPID TRANSFORMATIONS IN MEMBRANE FUSION.

How do two membranes, or two lipid bilayers, merge into one? First the two contacting (inner) monolayers merge into a structure called a stalk. Then the center of the stalk opens to allow the two outer layers to become a bilayer--called a hemifusion. Finally a toroidal pore has to form in this bilayer to complete the merger. The problem of membrane fusion is to understand how the potential barriers at each stage of transformation are overcome by the actions of proteins. In the last few years, we examined the X-ray diffraction of osmotically pressured membrane layers and discovered the intermediate stalk structure (Yang and Huang, 2002) and a pre-stalk membrane-in-contact intermediate state (Qian and Huang, 2012). These structures clearly show that the potential barrier for making contact and merging of two inner monolayers are each overcome by compressive force on the two membranes exerted by the fusion proteins.

Much less clear is the potential barriers for the transformation from the stalk state to full fusion. To investigate this problem, we focused on the endoplasmic reticulum (ER) fusion protein atlastin. Atlastin is distinct in having a V-shaped transmembrane domain (TM) and a cytosolic C-terminal tail. We are reconstituting atlastin into giant lipid vesicles (GUVs). We have developed a fusion assay by using GUVs, where, from the shape change of the GUVs, it is possible to measure the free energy changes at various stages of fusion transformations (Sun, Lee and Huang, 2011).

RANDALL G. HULET, C-1133, Rice University. **MATTER WAVE SOLUTIONS: COLLISIONS, COHERENCE AND ATOM INTERFEROMETRY.**

Solitons are localized wave disturbances that propagate without changing shape, a result of a nonlinear interaction which compensates for wave packet dispersion. Solitons are a ubiquitous wave phenomenon, occurring in optics, water waves, and in many diverse phenomena, perhaps even in the collective oscillations of protein and DNA molecules. We study matter-wave solitons created from Bose-Einstein condensates of ultra-cold atoms, with an attractive atom-atom nonlinear interaction. We exploit the ability to finely tune and manipulate ultra-cold atomic gases to explore soliton collisions at a level of detail that has not been previously possible. We report a detailed experimental study of how solitons pass through one another, while at the same time, exhibiting a complex collisional behavior. We show that the nature of the collision is governed by the relative phase and explore the cross-over from the 1D to 3D regime, where collisions result in annihilation or merger.

We have also characterized the Feshbach collisional resonance in ^7Li by associating ultra-cold atoms into very weakly bound molecules. This work enabled us to study the 3 and 4-body "Efimov molecules" that were predicted to occur in strongly interacting atomic gases.

Finally, we have also created a model for high-temperature superconductors using ultra-cold spin-1,4 atoms in an optical lattice. We observed that the atoms form an antiferromagnetic phase, similar to the cuprate superconductors.

SIMON B. HUMPHREY, F-1738, The University of Texas at Austin. **NEW POLY-CARBOXYLATED ARYL PHOSPHINES FOR THE DESIGNED SYNTHESIS OF COORDINATION COMPLEXES AND POLYMERS.**

In the past grant year, we have continued to successfully discover and report new research findings that have arisen directly from the core aims outlined in the original grant proposal. Research in the 13/14 period has focused on three main themes: 1) the determination of reproducible routes for the preparation of previously unknown asymmetric phosphine ligands with carboxylic acid functional groups, for use in the construction of coordination polymer materials with desired network topologies; 2) the preparation and characterization of new phosphine coordination materials (PCMs) using new ligands, *via* conventional and previously unstudied microwave-assisted methods; 3) the application of phosphine ligands and newly-determined microwave-assisted chemistry to the construction of unusual metallic nanoparticle catalyst materials. We have successfully published in each of the above areas in the past year, and other works are also pending at the time of writing.

New synthetic routes have been determined for the preparation of poly-carboxylated chelating phosphine ligands - namely *bis*(phosphines) and so-called PCP-pincer ligands. These types of ligand have been used to prepare metalated organometallic complexes; the complexes are interesting in their own right as water-soluble analogues of other well-known homogeneous catalysts. We have made a major breakthrough in our overarching aim, to prepare crystalline, ordered polymer frameworks using such molecules, and this work was highlighted as a communication in *JACS*. On the back of this important preliminary result, we have recently prepared several other related materials, which will be reported in the coming grant year.

Meanwhile, research involving mono-phosphine ligands has also leapt forward in the past year, with the realization of means to prepare large amounts of materials in a fast, economical and environmentally-benign manner using water as the only solvent, with microwave-assisted heating. We have also demonstrated in a full paper published in *Inorg. Chem.* that our PCMs display possibilities for an unprecedented number of post-synthetic modifications, which allows for broad tuning of the solid-state properties of a single material.

A porous Co_3O_4 -based material whose synthesis was reported in the previous grant year was revisited in the past twelve months. Collaborative studies with the Mullins group at U.T. Austin have focused on the use of our materials as potential Li and Na ion battery materials. The results of this study have been compelling, showing the extreme stability of these solids after hundreds of charge-discharge cycles. This work was very recently reported in *J. Mat. Chem.*

Based on the above results, we have a very clear vision for our research activities in the next two years, which will capitalize on these significant abovementioned breakthroughs.

GYEONG S. HWANG, F-1535, The University of Texas at Austin. **FIRST-PRINCIPLES INVESTIGATION OF THE STRUCTURE, CHEMISTRY AND PROPERTIES OF GRAPHENE-BASED NANOMATERIALS.**

Graphene-based materials have been proposed as promising electrodes for electric double layer capacitors. Recently, it has been found that one of the limitations of graphene electrodes is the finite quantum capacitance at low applied voltage. We investigated the impact of having point-like topological defects in graphene on the electronic structure and quantum capacitance using first-principles calculations. Our results clearly show that the presence of defects, such as Stone Wales, Di-vacancies, and di-interstitials, can substantially enhance the quantum capacitance when compared to pristine graphene, which is found to be due to defect-induced quasi-localized states near the Fermi level. In addition, the charging behavior tends to be asymmetric around the neutrality point. Furthermore, our work demonstrates the possibility of tuning the electronic structure and capacitance through mixtures of these defects. Our findings highlight that graphene electrodes with topological defects can be used to enhance the overall capacitance of supercapacitors by virtue of the increased quantum capacitance. Our study also suggests that graphene-based electrodes can be specifically tailored as separate positive and negative electrodes, which could significantly enhance the performance of supercapacitors.

TATYANA I. IGUMENOVA, A-1784, Texas A&M University. **A NOVEL INTERACTION WITHIN PROTEIN KINASE C ENZYME.**

Significant progress has been made towards Objective 2 of the proposal. We have:

- (1) Established that Ca^{2+} pre-binding to the C2 domain enhances the C2-V5 interactions. In the process of investigating Cd^{2+} as a potential Ca^{2+}

surrogate, we found that although Cd^{2+} binds tightly to the C2 domain, it does not promote the association of C2 with phospholipid membranes (published in *JACS* in 2013).

(2) Obtained the structure of the C2-V5 complex using NMR restraints-driven docking approach. The structure, which is currently being refined, revealed for the first time the atomic-level information about the interface between the two domains. The interface is stabilized by electrostatic interactions between the phosphate group of the V5 hydrophobic motif and the lysine-rich cluster of C2, as well as salt bridges, stacking of aromatic rings, and cation- π interactions. The C2-V5 work has been presented at the Biophysical Society meeting (talk) and SWRM ACS meeting (poster), and is being prepared for submission.

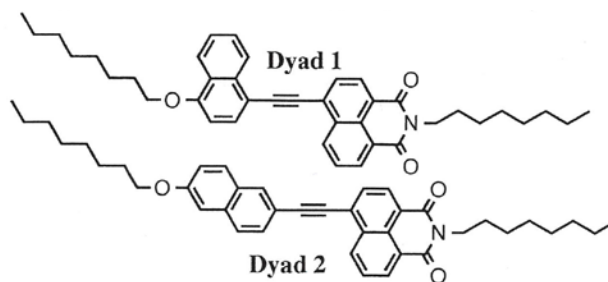
(3) Developed a novel application of paramagnetic lanthanide ions to structural biology of PKC, by using the native metal ion-binding site of the C2 domain and detecting the pseudo-contact shifts (PCS) on V5. The PCS restraints will be incorporated into the refinement protocol of the C2-V5 complex.

(4) To lay the foundation for probing V5 interaction with other PKC domains, conducted NMR studies of the C1B domain (submitted to *JBC*) and developed the purification and over-expression protocols for the full-length regulatory domain of PKC.

(5) Contributed our NMR expertise towards a collaborative project that focuses on a PIP_2 -binding protein (submitted to *Molecular Cell*).

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

An important emerging area of materials research concerns the synthesis and analysis of molecules that respond with a dramatic color change in response to stimuli such as heat or pressure. We have now thoroughly investigated the solution- and solid-state photophysical and stimuli-responsive properties of a series of aromatic conjugated donor-acceptor dyads represented by **dyad 1** and **dyad 2**. While **dyad 1** showed a difference in solid-state color between relatively faster (yellow) and slower (orange) evaporation from solution, **dyad 2** only showed one color (yellow-green) for both evaporation rates. Both dyads exhibited bathochromic solvatochromism as a function of increased solvent polarity with fluorescence quantum yields that decreased upon going from non-polar (*n*-hexane) to polar (acetone) solvents. Powder XRD and DSC were used to confirm the presence of two polymorphs of **dyad 1**. Remarkably, **dyad 1** demonstrated thermochromic, mechano-chromic and vapochromic stimuli-responsive behavior and was capable of switching between orange and yellow colors in the solid-state upon cycles of heating or applied pressure and vapor-fuming. To our knowledge, we have also recorded the first detailed images of a thermochromically and mechochromically-driven solid-solid transition in a single crystal. Detailed structural characterization confirmed the orange form as having a head-to-head stacked arrangement in the crystalline state, while the yellow form is composed of a head-to-tail stacked arrangement in a kinetically stable mesophase. The ability of **dyad 1** to 1) show three types of stimuli-responsive behavior in the solid-state and 2) show solution-state emission changes with solvents of varying polarity makes it a unique molecule. We are currently investigating its possible use in sensors, polymers and other applications.



MAKKUNI JAYARAM, F-1274, The University of Texas at Austin. COMPLEX ACTIVE SITES FOR PHOSPHORYL TRANSFER: CONTINUED CHEMICAL, BIOCHEMICAL, BIOPHYSICAL AND STRUCTURAL ANALYSES.

A. Stereochemically pure synthetic DNA substrates containing methylphosphonate (MeP) substitution were utilized to characterize the stereochemical preferences of wild type Cre and Flp as well as their derivatives containing point mutations in their catalytic pentad positions. The wild type recombinases and variants lacking one of the arginine duos of the catalytic pentad show a strong S_F preference. The variants lacking the second arginine have no preference or slight R_F preference. Lack of each of the other three pentad residues modulates the preference in specific ways. This work completes one of the main objectives of the present grant. **B.** Using single molecule tethered particle motion (smTPM), we have made considerable progress in understanding the kinetic and thermodynamic contributions of individual residues of the catalytic pentad towards each of the pre-chemical steps of recombination. **C.** The results from a combined difference topology and single molecule FRET analysis of the organization of DNA partners within the recombination synapse formed by the Flp has been published recently in *J Mol Biol*. **D.** By directed evolution, we developed Flp variants with specificity for native sequences that occur within the human genome. Experiments to test the ability of these variants to perform targeted genetic rearrangements in human cells are in progress. **E.** We have found that a reporter plasmid (generated by site-specific recombination) containing a specific partitioning' sequence interacts with a nuclear motor that engages and moves chromosomes during yeast meiotic cell division. The plasmid thus gains access to telomeres and accomplishes chromosome-like segregation. The findings have implications for the chromosome-associated propagation of selfish DNA elements, including certain mammalian viruses during latent infection.

JEAN X. JIANG, AQ-1507, The University of Texas Health Science Center at San Antonio. IDENTIFICATION OF SODIUM AND GLUTAMINE BINDING OF SNAT1 AMINO ACID TRANSPORTER USING MATAGENSIS SCANNING APPROACH.

SNAT1 is a member of system N/A amino acid transport family that primarily expresses in retina and neuron, and mediates the transport of L-glutamine. To use SCAM approach to determine the critical residues involved in sodium and L-glutamine binding, we need to first mutate all endogenous cysteines. Mutation of the two highly conserved residues Cys-249 and Cys-321, compromised the transport function of SNAT1. However, this reduction was not caused by the decrease of SNAT1 on the cell surface since the cysteine-null mutant generated by replacing all 8 cysteines with alanine was equally capable of being expressed on the cell surface as wild-type SNAT1. Interestingly, by retaining two cysteine residues, 249 and 321, a significant level of L-alanine uptake was restored, indicating the possible formation of disulfide bond between these two conserved residues. Biotinylation crosslinking of free thiol groups with MTSEA-biotin provided direct evidence for the existence of a disulfide bridge between Cys-249 and Cys-321. Together, these results suggest that cysteine residues 249 and 321 form a disulfide bridge, which plays an important role in substrate transport but has no effect on trafficking of SNAT4 to the cell surface.

JIN JIANG, I-1603, The University of Texas Southwestern Medical Center. STUDY OF CHEMICAL MODIFICATION IN CELL SIGNALING.

The secreted proteins of the Hedgehog (Hh) family play pivotal roles in embryonic development and adult tissue homeostasis. Abnormal Hh pathway activity leads to numerous human disorders including cancer. We obtained evidence that the SUMO pathway regulates Hh signaling and identified the Hh signal transducer Smoothed (Smo), a seven transmembrane protein of the GPCR family, as a SUMO substrate. We found that Smo is SUMOylated in response to Hh stimulation, and that Smo SUMOylation regulates its trafficking and cell surface expression by antagonizing its ubiquitination. SUMOylation deficient Smo variants exhibited increased ubiquitination and decreased stability *in vitro* and comprised activity *in vivo*. We found that Hh stimulates Smo SUMOylation by dissociating the desumoylation enzyme Ulp1 from Smo, and that SUMOylation recruits a deubiquinating enzyme UBPY to antagonize Smo ubiquitination. Thus, our study has established a new paradigm for exploring the antagonistic relationship between SUMOylation and ubiquitination in the regulation of a membrane receptor. We further showed mammalian Smo is also SUMOylated in response to Sonic Hedgehog stimulation. We are in the process of determining whether SUMOylation of mammalian Smo is critical for its ciliary localization and signal transduction.

NING JIANG, F-1785, The University of Texas at Austin. ERROR-FREE HIGH-THROUGHPUT GENE SEQUENCING.

During the second year of the Welch support, we have developed a molecular barcoded immune repertoire sequencing methods (MBCIRS). This method demonstrated superior robustness in handling various cell input amount, a hundred fold reduction in the error rate, and reduce bias created by PCR. We have used this method and tested naïve B cells sorted to different amount, from as few as 1,000 to as many as 1,000,000. Results showed that there is a good correlation between the cell number and antibody heavy chain diversity detected. We have submitted the manuscript to Nat Methods. We are currently using the technology to study somatic hypermutations in the antibody repertoire in malaria patients to further test the power of quantitative and accurate sequencing bring to the immune repertoire analysis.

One of our collaboration with Yuan Zhuang's group at Duke University that examines the TCR gene usage in the invariant natural killer T (iNKT) cell development was published in the *Journal of Immunology*.

QIU-XING JIANG, I-1684, The University of Texas Southwestern Medical Center. STRUCTURAL BASIS FOR THE LIGAND-GATING OF A TYPE 1 IP₃ RECEPTOR.

We made three major discoveries. 1) We have been improving our preparation of IP₃Rs for structural studies at high resolutions. We have successfully made recombinant IP₃Rs, and started working on implementing the new chemical engineering technology to conduct spherical reconstructions of IP₃Rs in membranes. The recent breakthrough in the technology of direct electron detector makes it important to combining the high-end instrument with a new detector in order to improve resolutions. The conformational flexibility of the IP₃Rs is a potential limit and putting the receptors into membrane environment is a good alternative to overcome this problem. 2) The study of the chromogranin B (CHGB) led to the new finding that CHGB forms a novel ion channel in membranes, and its concentrated binding can shape the membranes into tubular shapes with high curvature. We have characterized the channels functions by three different methods, and have been studying the physiological importance of CHGB in the maturation of secretory granules in insulinoma cell lines. The structural study of CHGB by cryoEM and crystallography has been initiated as well. 3) The importance of CHGB in the metastasis of neuroendocrine tumor cells. It was a surprise that the transcription level and protein level of CHGB in metastatic pheochromocytomas (PCs) and paragangliomas (PGLs) were found to be significantly higher than in benign tumors. We are collaborating with Shay lab in understating the importance of CHGB to cancer survival in hypoxic environment.

YOUXING JIANG, I-1578, The University of Texas Southwestern Medical Center. STRUCTURAL AND FUNCTIONAL STUDIES OF RCK-REGULATED POTASSIUM CHANNEL.

Over the past year, we have identified a novel plant nucleolus membrane channel DMII (also named Castor or Pullux) that plays an essential role in the symbiosis between legumes and bacteria (*rhizobium*) or fungi (*arbuscular mycorrhizal*) for nitrogen fixation. We have structurally demonstrated that the channel functions as a tetramer and its C-terminal ligand binding domain of each subunit contains two tandem RCK domains just like the other RCK-regulated K⁺ channels. Interestingly, this channel is unlikely to be K⁺ selective. Our structural study also reveals multiple Ca²⁺ binding sites on each subunit, suggesting that the channel is regulated by Ca²⁺. We are now in the process of performing electrophysiological analysis of the channel to define the selectivity and gating

properties of this dual RCK-containing, ligand gated channel.

Part of Welch funding was diverted to support the study of the ion selectivity mechanism of K⁺ channels using non-selective NaK channel and its mutants as the model systems. To visualize how K⁺ out-competes Ne in the filter of the K-selective channels, we have recently performed a crystallographic titration on NaK2K, a K⁺ selective NaK mutant, and demonstrated that K⁺ binding at the four seemingly identical sites of the K⁺ channel filter is not equivalent at low K⁺ concentrations. At high K⁺ concentrations (150 mM) two K⁺ ions evenly occupy the four sites in the selectivity filter, whereas in a low K⁺/high Na⁺ environment (1 mM K⁺/149 mM Na⁺) a single K⁺ ion remains bound in the selectivity filter; preferably at sites 1 or 2 in NaK2K. This study was recently published on *Nature Communications*. In addition, we have also structurally characterized the binding profile of Rb⁺, Cs⁺ and Ba²⁺ in NaK2K filter and provided structural insights into the so-called Ba²⁺ lock-in phenomenon in K⁺ channel. This study was recently published on *JGP*.

JIN JIANPING, AU-1711, The University of Texas Health Science Center at Houston. DISSECTION OF MECHANISMS FOR POLYUBIQUITIN CHAIN SYNTHESIS.

Linear polyubiquitin chain is important for NE-κB activation and inflammation response. Recent studies indicated that linear polyubiquitin chain is important for cell survival as well. However, the mechanism by which the LUBAC ubiquitin ligase synthesizes linear polyubiquitin chains is still unclear. In this proposal, we will determine how linear polyubiquitin chain is produced by different pairs of E2 and E3 enzymes and analyze the roles of E3 and ubiquitin surface residues in linear polyubiquitin chain formation. In the second year of our research, we are continuing our efforts to purify all three subunits of the LUBAC ubiquitin ligase using different expression systems. With all three subunits purified, we put more efforts to assemble the entire LUBAC complex. We have also purified the C885A mutant of HOIP using baculovirus system. Now we have assembled the inactive LUBAC complex with the C885A mutant of HOP as well. With these reagents in hands, we are developing *in vitro* assays to synthesize linear poly-ubiquitin chains. We have purified UbcH7 and UbcH5C using bacteria expression system. We found that UbcH7 has methionine reactivity. Furthermore, we have purified seven alanine mutants of surface residues of ubiquitin. We will test their functions in the synthesis of linear polyubiquitin chains by the LUBAC complex in the third year.

KENNETH A JOHNSON, F-1604, The University of Texas at Austin. KINETICS OF NUCLEOTIDE BINDING BY HIV REVERSE TRANSCRIPTASE.

We are just completing four papers describing detailed kinetic analysis of mutants of HIV RT that are resistant to nucleoside analogs. In particular, we have quantified the kinetics of nucleotide binding, enzyme conformational changes and rates of chemistry to define the effects of each mutation on the incorporation of normal nucleotides compared to the corresponding nucleoside analogs. We have also measured the kinetics of ATP-dependent excision of chain terminators such as AZT, a reaction which was thought to be the major basis for resistance to AZT. In our quantitative analysis, we show that ATP-dependent excision only accounts for a factor of five toward the resistance to thymidine analogs, while other steps in the pathway (DNA translocation, binding of the next correct base pair) contribute as much or more to the resistance pattern. Because our conclusions run against the current dogma in the field, we have postponed publishing our results until we can simultaneously publish all of our papers that unequivocally define our new paradigm for understanding resistance. This grant has also supported a pilot project to begin studies on the human mitochondrial DNA polymerase, which is the target for toxic side effects of nucleoside analogs. In a recently published paper (Qian et al, *JBC* 2014), we described how we can replace the yeast mitochondrial DNA polymerase with the human enzyme and then use the yeast system to examine the effects of mutations in the human mitochondrial DNA polymerase and thereby relate our solution kinetic studies to the physiological effects seen in yeast. This study has provided the preliminary results forming the basis for a new grant application submitted to NIH.

KEITH P. JOHNSTON, F-1319, The University of Texas at Austin. TUNING NUCLEATION NANOCLUSTERS ASSEMBLED FROM PRIMARY NANOPARTICLES.

Gold plasmonic nanoclusters composed of primary particles were synthesized by colloidal assembly to achieve strong absorbance in the near infrared region. The charge on the primary particles was modified with pH, salinity and ligands on the particle surface to tune the assembly, as guided by a model based on statistical mechanics. Small angle X-ray scattering was used to determine the spacing of the primary particles as a function of the colloidal interactions that drive the assembly and the nature of the ligands on the particle surface. The viscosity of dispersions of proteins was examined as a function of the nature of the colloidal interactions, which were tuned by adding various small molecules. In a study of iron oxide nanoclusters coated with copolymers, the interaction of the particles with various substrates was investigated at very high electrolyte concentrations. The transport of the particles in porous media was related to the strength of these interactions. A new chemical mechanism has been identified where perovskite oxides undergo room temperature anion intercalation pseudocapacitance for fast energy storage. In contrast, previous studies have focused on cation intercalation. Furthermore, electrocatalytic activity of perovskites has been tuned through active site variation to examine pathways for the oxygen evolution reaction and oxygen reduction reaction. In each case the materials were designed by colloidal synthesis concepts to control the morphology.

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

We have continued to make progress in the two main areas focused on the study of molecular precursors to functional materials. We have now published our studies on the use of mononuclear precursors for the chemical vapor deposition (CVD) of thin films of amorphous Co and Co alloy films. We have made significant progress in our studies on large polynuclear complexes of the lanthanides, especially with regard to the development of materials which have promising emissive photophysical properties. A major review of some of our work in this area has appeared in *Coordination Chemistry Reviews*. We

have also published our studies on a linear hexanuclear Yb salen complex with enhanced near-infrared (NIR) luminescence and, for example, heterotetranuclear Zn_2Ln_2 complexes of Nd, Yb and Er with a benzimidazole based ligand system. We also reported initial studies on NIR luminescent poly methyl methacrylate (PMMA)-supported metallopolymers based on Zn–Nd Schiff-base complexes. Thus, Schiff-base ligands H_2L^1 (N,N'-bis(5-(3'-vinylphenyl)-3-methoxy-salicylidene)ethylene-1,2-diamine) or H_2L^2 (N,N'-bis(5-(3'-vinylphenyl)-3-methoxy-salicylidene)-phenylene-1,2-diamine) react with $Zn(OAc)_2 \cdot 2H_2O$ and $Ln(NO_3)_3 \cdot 6H_2O$ in the presence of pyridine (Py) to give two series of hetero-binuclear Zn–Ln complexes $[Zn(Ln)(Py)Ln(NO_3)_3]$ ($n = 1, Ln = La, Nd, Gd$, or $n = 2, Ln = La, Nd, Gd$). These complexes produce PMMA supported hybrid materials by controlled copolymerization with methyl methacrylate. The Nd containing materials exhibit strong and characteristic near-infrared (NIR) luminescent Nd^{3+} -centered emissions.

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

One goal of our research is to unify descriptions of porphyrin, corrole 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. To help accomplish these goals we continued to elucidate the electrochemistry, spectroelectrochemistry and electrocatalytic activity of different series of macrocycles containing multiple interacting or non-interacting redox centers. A large number of compounds were investigated over the last 12 months. Examples include: 1) hydroxyl-substituted free-base tetraphenylporphyrins, 2) tetraarylporphyrins containing nitro-substituents on the β -pyrrole positions of the macrocycle, 3) homo and heterobimetallic pyrazinoporphyrazines, 4) tetrabenzocorroles functionalized with different electron-withdrawing groups on the β,β' -fused rings, 5) π -extended porphyrins bearing an electron-rich naphthalene moiety, 6) β -phosphorylated porphyrins, 7) open-chain pentapyrroles and the corresponding sapphyrins, 8) planar and nonplanar free-base β -pyrrole substituted *meso*-tetraarylporphyrins, 9) cobalt(III) and cobalt(II) triarylcorroles containing 0-3 nitro groups on the *para*-position of the three *meso*-phenyl rings of the macrocycle and 10) a tetra-ruthenium complex containing two ruthenium(II) phthalocyanines and one metal-metal bonded diruthenium(III, III) unit. In addition to the above, we expanded our studies involving electrosynthesis of π -extended porphyrins to include a series of Zn(II), In(III), Ir(III) derivatives, as well as expanded our studies of electrocatalysis to include the electroreductive dechlorination of α -hexachlorocyclohexane by iron porphyrins. Finally, we initiated a detailed examination of protonated and deprotonated free base porphyrins in nonaqueous media.

CRAIG D. KAPLAN, A-1763, Texas A&M University. BIOCHEMICAL AND BIOPHYSICAL DETERMINATION OF CONSERVED RNA POLYMERASE DOMAINS FUNCTION IN CATALYSIS, ABORTIVE INITIATION AND TEMPLATE INTERACTION

First and foremost, we have brought our studies on the catalytic activities of WT yeast RNA Polymerase II and a catalytically deficient mutant (Rpb1 His1085Tyr), described in the previous progress report, to publication. This was a substantial amount of work and a major goal of our previous funding period. This paper describes a novel activity of His1085Tyr RNA Polymerase in yeast that is gained upon mutation of the essential and conserved "trigger loop" domain of the RNA Polymerase II active site. This activity was wholly unexpected and describes a novel RNA cleavage mode for RNA Polymerase II. The rest of our results on this project were described in our previous progress report, however, we needed to generate a number of repeats of data described in previous report, write and edit the manuscript and proceed through submission and review.

We have also reported exceptionally interesting results in collaboration with Dr. David Schneider at U. Alabama-Birmingham about comparatively biochemistry of RNA Polymerases I and II (Pol I and Pol II). We have found that mutations in trigger loop residues absolutely conserved between Pol I and Pol II (E1103G in Pol II, E1224G in Pol I) have different biochemical outcomes on their respective polymerases, but these outcomes are conditional relative other residues within the trigger loops. Our model is that Pol I and Pol II have different rate-limiting steps in their transcription cycles, in one case catalysis appears to be limiting, in the other translocation on the DNA template appears to be limiting. Certain trigger loop mutants alter these two steps in opposing fashion, and thus an identical change in one enzyme can appear to be inhibit activity while in another enzyme, the same change promotes activity. We showed that additional mutations in Pol I that are presumed to cause catalysis to be limiting allow E1224G to exert a positive effect in this background just as E1103G does to otherwise wild type Pol II, in contrast to E1224G behavior in otherwise wild type Pol I.

We also report our contributions to work from the Engelke lab (U. Michigan) on the inhibition of Pol II by unstructured RNAs, and with the Block and Kornberg labs (Stanford University) on the functions of TFIIF and TFIIS in single molecule studies of Pol II. This work is especially important because it contradicts other recent work published in *PNAS* on a similar topic from a competing group. The experimental setup and experimental details in our paper allowed more nuanced conclusions regarding mechanisms by which the factors TFIIF and TFIIS alter elongation properties of Pol II. This makes this work significant.

ADRIAN T. KEATINGE-CLAY, F-1712, The University of Texas at Austin. PREPARATIVE *IN VITRO* BIOSYNTHESIS OF COMPLEX POLYKETIDES.

Our lab continues to learn about the enzymology of modular polyketide synthase enzymes in our quest to employ them in the synthesis of valuable chiral compounds. Click chemistry was used to probe the reactivities of a polyketide synthase module (Hughes et al., 2013). We learned that the inexpensive handle, ethanethiol, can be used (instead of more CoA-like moieties) for both priming and extender units when employing modules in the biocatalytic synthesis of triketide building blocks. Dehydratases, α -ketoreductases, and enoyl-isomerases have been added to our arsenal of biocatalytic enzymes (Gay et al., 2013; Piasecki et al., 2014; Gay et al., 2014b). Each of the crystal structures of these enzymes were informative about their function; however, we learned the most from the structure of a ketosynthase covalently bound to its polyketide substrate (Gay et al., 2014a, *cover of *Structure*). The gatekeeping activity of ketosynthases is important to decipher so that modular polyketide synthases may be more reliably engineered. We are also about to submit our studies of a

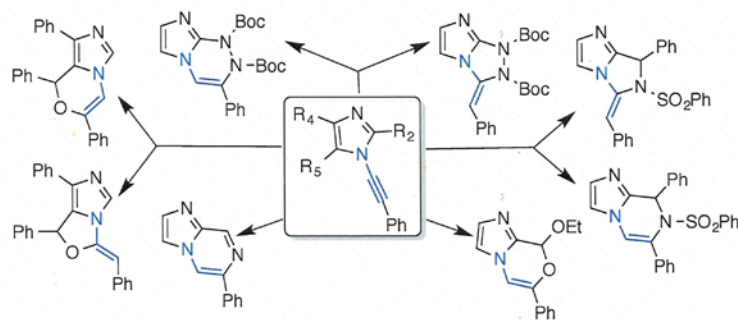
related carbon-carbon bond-forming thiolase that we are employing biocatalytically on N-acetylcysteamine-bound substrates. A new postdoc, David Stevens (from the Richard Taylor lab) will join us this August to perform several biocatalytic studies pertaining to this grant.

KEVIN F. KELLY, C-1605, Rice University. INVESTIGATING THE NANOSCALE SURFACE CHEMISTRY OF GRAPHENE.

Over the past decade, we have been applying our expertise in scanning tunneling microscopy to understanding the chemistry of atoms, molecules, and materials in two-dimensional systems. Among the many systems we have explored, we have had a great deal of success probing the chemical properties of graphene in both bulk and nanoparticle form. We have also used these graphitic surfaces as templates to pattern self-assemble monolayers of poly-3-hexylthiophene. Our new research involves a closer looker at the chemical preparation of the copper substrate prior to graphene growth. The tunneling microscope images provide information of the quality of the graphene film along with its relation to the underlying copper facet of the polycrystalline foil onto which it had grown. We also plan on continuing our nanoscale investigations into polymer self-assembly and ordering. Recently, we have found that the addition of the right amount of octanedithiol to the dissolved polymer mixture resulted in more linear and closer packed monolayers. This is an intriguing result and an area where we hope that by varying both the length of the alkane chain additive as well as varying the type and number of sulfur groups it contains will lead us to a more fundamental understanding of this phenomenon. Lastly we will apply this experimental expertise to other novel two-dimensional compounds, including such transition metal dichalcogenides as tantalum disulfide and titanium diselenide. In addition, we have coupled these studies with new work in compressive optical microscopy which as proof of its utility we have used to understand the plasmon resonances in gold nanobelts through high-speed dark-field imaging. Base on this, we are building a compressive imaging Raman microscope system to gain more detailed chemical information on these systems.

SEAN M. KERWIN, F-1298, The University of Texas at Austin. REARRANGEMENTS OF ALKYNYLIMIDAZOLES.

The versatile role of *N*-alkynylimidazoles as synthons for the rapid construction of a wide range of heterocycles has been demonstrated. In one recent example, we demonstrate that intramolecular hydroalkoxylation and hydroamination reactions proceed with very high or complete control of regiochemistry to afford synthetically useful yields of either the products of *5-exo-dig* or *6-endo-dig* cyclization, depending upon reaction conditions (Scheme 1). The high degree of regiocontrol in these diverse systems highlights the unique electronic features of these *N*-alkynylimidazoles, and sets the stage for application of these cyclizations in the construction of more complex synthetic targets.



Scheme 1. Examples of regiocontrol in the cyclizations of *N*-alkynylimidazoles.

CHING-HWA KIANG, C-1632, Rice University. SINGLE MOLECULE STUDIES OF MOLECULAR INTERACTIONS OF BIOLOGICAL MACROMOLECULES.

Development of nanoscale distance and piconewton force measurements has allowed us to study single molecule dynamics of biological macromolecules, to gain insight into protein-protein, protein-nucleic acid, and protein-cell surface interactions. Using atomic force microscope force studies, we found that the multimeric von Willebrand factor (VWF), has two folded states that can be switched with mechanical forces, a key step in initiating platelet adhesion, and the existence of those metastable states depend on the multimer size. These results provide insight into the mechanism of mechanical activation of VWF, whose function is critical in initiating blood clotting. The results have been published in *Physical Review Letters*. We have also used Crook's fluctuation theorem to reconstruct the free energy landscapes of single-stranded DNA stretching transitions. We have combined imaging and force studies to study extracellular matrix proteins and their mechanical properties in solution. Such studies open a door for future investigation of multiscale systems including molecular-molecular, molecular-cellular, and cellular-cellular interactions.

CHONGWOO A. KIM, AQ-1813, The University of Texas Health Science Center at San Antonio. STRUCTURE OF AN EPIGENETIC REGULATORY COMPLEX.

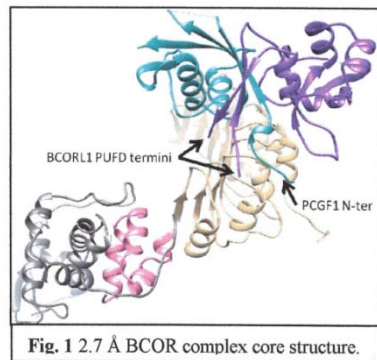
The main goal of my lab is to understand the structural basis of how multi-protein epigenetic complexes are assembled and understanding the gene regulatory consequences of their assembly mechanism.

The BCOR complex

Our major focus over this past year has been the study of a 10 component epigenetic complex called the BOOR complex. The four proteins that unite the two histone modifying activities of the BCOR complex, and thus the core, are PCGF1, BCOR, KDM2B and SKP1. As we had originally proposed to do, we have successfully determined the high resolution three dimensional X-ray crystal structure of the BCOR complex core (Fig. 1). As predicted from our binding studies, the structure confirmed hierarchical assembly of the BCOR complex which in turn likely coordinates the multiple histone modifying enzymatic activities of the complex.

Multiple SAM architectures

SAMs are protein modules that can polymerize forming the basis of higher order chromatin structures. We have determined that the SAM from PHC3 can form both a novel five and six repeat polymer structures. This suggests that PHC3 SAM polymers could form alternative higher chromatin states using the flexible SAM polymer. This work has been accepted for publication.



TAE-KYUNG KIM, I-1786, The University of Texas Southwestern Medical Center. BIOCHEMICAL CHARACTERIZATION OF A NOVEL CLASS OF NONCODING RNAS.

We have successfully verified the functionality of enhancer RNAs (eRNAs) in transcription by two independent knockdown approaches (shRNAs and Locked Nucleic Acid-modified antisense oligonucleotides) in two different cell types (Neurons and NIH3T3). Using these knockdown-based approaches and other biochemical assays, we were also able to identify a novel action mechanism of eRNAs during transcription induction. Briefly, we found that eRNAs promote the early transcription elongation of RNA polymerase II from neuronal immediate early genes by titrating away a negative transcription elongation factor, which pauses RNA polymerase II at the promoter-proximal region. Upon knockdown of eRNAs, the negative elongation factor remains bound to the target promoter even under activating condition, resulting in a decrease in transcription of target gene. Collectively, our study highlights the spatiotemporally regulated action mechanism of eRNAs during early transcriptional elongation. A manuscript describing our findings is currently under second review at *Molecular Cell*.

DOUGLAS J. KLEIN, BD-0894, Texas A&M University at Galveston. CHEMICAL MODELS: CLASSICAL TO QUANTUM-THEORETIC.

The development and application of a diversity of models for molecules and nano-structures continues, with connection to classical chemical ideas. First, interest continues in different topologically arranged nano-structures, especially for conjugated-carbon pi-networks, including: ordinary benzenoids, fullerenes, pi-network polymers, buckytubes, defected graphenes, nano-cones, and "super-polyhedra". Some attention continues to be directed to resonating valence-bond (VB) theory, including foundations for the models and also for E. Clar's "aromatic-sextet" ideas. Weak pairing of electrons (and consequent magnetic and electrical properties) for some novel nano-structures is being investigated, often utilizing our resonating VB ideas as well as conventional molecular orbital (MO) ideas. Fundamental topological-structural characterizations of dislocations and disclinations as decorations or defects in extended conjugated carbon-network species are being pursued, and developed, including in terms of both MO and VB theory. Further, progressive molecular reaction networks have been mathematically characterized as a type of partially ordered set, and associated theory has been and continues to be utilized, *e.g.*, to enable selected isomer enumerations and to interpolate/extrapolate molecular properties. Study continues of some novel borane and carborane based moieties with icosahedral cores, especially regarding nano-conglomerates of their monomers. Several related chemical graph-theoretic topics have been considered or are under consideration, especially involving novel chemistry or mathematics, which then is pursued.

STEVEN A. KLIEWER, I-1558, The University of Texas Southwestern Medical Center. CHARACTERIZATION OF THE ENDOGENOUS LIGAND FOR THE IMMUNOMODULATORY ORPHAN NUCLEAR RECEPTOR ROR γ .

ROR γ is an orphan nuclear receptor that is required for the differentiation and immune response of Th17 cells. A major focus over the past year has been the characterization of 22:4 lysophosphoethanolamine (LPE), which we purified from bovine thymus lipid extracts as an activator of ROR γ transcriptional activity. However, in ligand binding assays, LPE did not interact directly with ROR γ . Thus, we conclude that LPE activates ROR γ indirectly via a secondary mechanism. Efforts are underway to identify this pathway.

In a second project, we have developed a sensitive assay with which to detect the hormone FGF15 in blood. Based on genetic evidence, we proposed that FGF15 is released by small intestine to act on liver to regulate carbohydrate and lipid homeostasis. However, due to FGF15's poor antigenic properties, developing an assay with sufficient sensitivity to detect FGF15 in blood has proven difficult. We have now developed a stable isotope standard and capture by anti-peptide antibodies—selected reaction monitoring (SISCAPA-SRM) assay that combines immuno-enrichment with mass spectrometry to overcome this issue. Using this assay, we have shown that FGF15 circulates at low nanogram/milliliter concentrations, which are consistent with those

required for it to activate its receptor. We are currently using this assay to determine how FGF15 is regulated in response to various physiologic and pathophysiologic conditions including fasting/refeeding, diabetes and obesity.

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

Within the relaxation time approach using free nucleon-nucleon cross sections modified by in-medium nucleon masses that are determined from an isospin- and momentum-dependent effective nucleon-nucleon interaction, we have obtained a valley shape in the temperature or density dependence of the specific shear viscosity of neutron-rich nucleonic matter near its liquid-gas phase transition, with the steepness of the valley depending on the order of the phase transition. Using a partonic transport model, we have shown that including a vector mean field in baryon-rich quark matter leads to a splitting of the quark and antiquark elliptic flows. Including also hadronic mean fields in a hadronic transport model, we have found that observed elliptic flow differences between particles and their antiparticles at the Relativistic Heavy-Ion Collider is consistent with an appreciable vector mean field in the partonic matter. Based on a kinetic description of charmonium dissociation and production in the expanding quark-gluon plasma that is described by a 2+1 dimension ideal hydrodynamic model, we have found that the inclusion of hot medium effects gives a better description of the experimental data on charmonium production in p+Pb collisions at the Large Hadron Collider. Using a non-relativistic potential model, we have shown that including the full gluon wave function results in a reduction of the cross section for the leading-order gluon dissociation of charmonium calculated in the dipole approximation that is usually adopted in theoretical studies. Based on the QCD sum rule with its operator product expansion determined from lattice calculations for the pressure and energy density of hot QCD matter near the vicinity of the transition temperature between quark-gluon plasma and hadronic matter, we have found that the strength of the charmonium wave function at the origin decreases with temperature and follows exactly that obtained from the solution of the Schrodinger equation for a charm and anticharm quark pair using the free energy from lattice calculations as the potential and is in sharp contrast to that using the deeper potential associated with the internal energy.

JENNIFER J. KOHLER, I-1686, The University of Texas Southwestern Medical Center. NEW CHEMICAL TOOLS TO STUDY EXTRACELLULAR GLYCAN REMODELING BY SIALIDASES..

Aim 1 was to develop an assay to determine the glycan specificity of sialidases. We completed this aim (*ACS Chem Biol*, 2012). Using arrays of naturally occurring mammalian glycans, we are now using this method to determine the glycan specificity of three sialidases from *S. pneumoniae*. An additional publication in this area is anticipated in the upcoming year.

Aim 2 was to develop a method to discover the protein substrates of sialidases. Our strategy relies on an enzymatic reaction that can be used to oxidize terminal galactose residues and enable selective biotinylation of non-sialylated proteins. We used this method in combination with mass spectrometry to compare the non-sialylated proteins present on the surface of an untreated brain endothelial cell line, versus the same cell line that had been treated with one of three *S. pneumoniae* sialidases. We identified ~60 proteins that are substrates for these sialidases and confirmed the strongest hits. We are now working to determine whether *S. pneumoniae* bacteria desialylate the same substrates. In addition, we adapted the same chemical labeling/mass spectrometry method to discover the glycoprotein substrates of individual sialyltransferases. We discovered that the cancer-associated sialyltransferase ST6GAL1 sialylates and alters signaling through the tumor marker CDCP1. A manuscript describing these results is under review at *PNAS*.

During the previous granting period, we developed a method to incorporate a diazirine-modified form of O-GlcNAc into O-GlcNAc-modified proteins (*PNAS*, 2012). The methodology was limited because both the O-GlcNAc-transferase (OGT) and the O-GlcNAc hydrolase (OGA) had reduced activity toward diazirine-containing substrates. To improve the method, we identified a mutant OGA that is active toward diazirine-containing substrate (*MedChemComm*, 2014) and a mutant OGT that prefers diazirine-modified substrate (manuscript in preparation).

ANATOLY B. KOLOMEISKY, C-1559, Rice University. THEORETICAL UNDERSTANDING OF CHEMICAL MECHANISMS OF SELECTIVITY IN TRANSPORT THROUGH CHANNELS.

We developed a new theoretical method for evaluating properties of complex chemical systems. All chemical phenomena can be viewed as network of states connected by dynamic transitions. It is based on a hypothesis that distributions of events between two arbitrary states contain full information on mechanisms and dynamic properties of the system. The approach utilizes first-passage theoretical analysis, and exact arguments for any general network are presented. Using this method various systems are analyzed explicitly and the method is illustrated on several examples of complex chemical and biological processes.

We also studied complex chemical dynamics of cytoskeleton biopolymers such as actin filaments and microtubules. Using discrete-state stochastic models, which are solved analytically, we present a comprehensive physical-chemical analysis of hydrolysis processes in these filaments. Our approach naturally explains experimentally observed cooperativity phenomena, and theoretical predictions are also fully supported by Monte Carlo computer simulations. In addition, we investigated physical-chemical foundations of protein-DNA interactions in the process of protein search for specific sequences on DNA. We discuss a speed-selectivity paradox, which argues that the protein-DNA interactions must be simultaneously smooth to speed up the process and rough to support the selectivity of the special sites. Our theoretical analysis shows that the speed-selectivity paradox does not exist. It is just an artifact of using approximate continuum theoretical models for analyzing protein search in the region of the parameter space beyond the range of validity of these models. The method allows us to explain experimentally observed fast target search at the level of single molecules. Extensive Monte-Carlo computer simulations support our theoretical predictions.

JUNICHI KONO, C-1509, Rice University. OPTICAL, INFRARED, AND TERAHERTZ DYNAMICS OF CARBON NANOMATERIALS.

During the past year, we have made significant progress in several projects, including: i) *Plasmonic Nature of the THz Conductivity Peak in Single-Wall Carbon Nanotubes*. Plasmon resonance is expected to occur in carbon nanotubes in the THz range, but its convincing identification has been elusive. Here we performed THz measurements on enriched metallic and semiconducting nanotube films. A broad and strong THz conductivity peak appeared in both types of films, whose behaviors are consistent with the plasmon resonance explanation. ii) *Ultrafast Generation of Phonons in Enriched (6,5) Single-Wall Carbon Nanotubes*. Using a macroscopic ensemble of enriched (6,5) carbon nanotubes, we generated phonons in an ultrawide range (10–3000 cm⁻¹). A total of 14 modes were resolved, including fundamental modes and their combinational modes. Through comparison with calculations based on an extended tight-binding model, we were able to identify all the observed peaks and determine their frequencies. iii) *Carbon Nanotube THz Detector*. We have developed a powerless, compact, broadband, flexible, large-area, and polarization-sensitive carbon nanotube THz detector that works at room temperature. The detector is sensitive throughout the entire range of the THz technology gap, with responsivities as high as ~2.5 V/W and polarization ratios as high as ~5:1.

BRIAN A. KORGEL, F-1464, The University of Texas at Austin. NANOMATERIALS OF EARTH ABUNDANT ELEMENTS FOR ENERGY STORAGE AND HARVESTING.

A new synthetic route to silicon nanorods was discovered that did not require the use of pie-synthesized tin seed particles to induce solution-liquid-solid (SLS) growth. Trisilane, which serves as the reactant and silicon source in the reaction, was found to reduce the tin reactant to tin metal during the reaction to enable a single-step reaction for silicon nanorods. This new approach to silicon nanorod synthesis further simplifies the ability to make these unique nanomaterials. Tin-seeded silicon nanowires were tested in lithium ion batteries—both in coin cells cycling against lithium metal and by *in situ* transmission electron microscopy to directly observe lithiation and delithiation in real-time for individual nanostructures—and found to offer significantly enhanced rate capability in lithium ion batteries. These new materials provide a source of silicon that has extremely high charge storage capacity of lithium (nearly ten times greater than commercially-used graphite) with excellent performance at high charge and discharge rates. Silicon typically has poor electrical conductivity and slow lithiation rates, but the addition of significant amounts of tin into the nanowires yields dramatic improvement in these properties. Silicon nanocrystal synthesis was also further improved to yield highly uniform nanocrystals suitable for the formation of superlattices. The first example of a binary nanocrystal superlattice (BSL) with silicon nanocrystals was formed, combining silicon nanocrystals with gold nanocrystals.

DONALD J. KOURI, E-0608, University of Houston. SUPERSYMMETRIC QUANTUM MECHANICS: ACCURATE EXCITED STATE ENERGIES AND WAVE FUNCTIONS.

We explored potential uses of the supersymmetric quantum mechanical formulation for improving the accuracy and computational efficiency. In a paper (2013), we demonstrated a method for avoiding the computationally intensive fact that the SUSY-QM leads to a second sector Hamiltonian that is a tensor, with dimensions determined by the number of spatial variables, and showed that all calculations can be done with scalar Hamiltonians, reducing the required computing effort by orders of magnitude (non-Fermionic). We developed new ways to use the SUSY-QM formalism for applications to analysis of experimental data (by exploring the connection between SUSY-QM, the Heisenberg Uncertainty Principle and Fourier analysis). The result was generalization of the Fourier Transform and huge reductions in the minimum uncertainty product for time, frequency and space/wave number! (Uncertainty limit cut to 1/3 rather than 1/2, and are working to further reduce it.) We demonstrated the higher simultaneous resolution in time and frequency by analyzing field data from micro-seismic processes and obtained very high time-frequency resolution, correctly identifying the arrivals of the pressure and two types of shear waves. Polarization analysis of the arriving waves verified the results. Also, we considered the inverse scattering problem for acoustic scattering with the aim of determining the velocity contrast causing the scattering, extending the method from acoustic scattering to quantum scattering inverse problems. Our approach solved the "phase problem" of quantum (and electromagnetic) inverse scattering, which arises because the physical observable is the absolute square of the (complex) differential scattering amplitude. We are hiring a new postdoc this grant year to transfer our approach to quantum scattering.

LÁSZLÓ KÜRTLI, I-1764, The University of Texas Southwestern Medical Center. SYNTHESIS OF COMPLEX NATURAL PRODUCTS VIA NOVEL C-C BOND-FORMING PROCESSES.

During the third grant year we have developed three distinctly green (i.e., environmentally friendly) methods that do not need any transition-metal (TM) catalyst. First, we found that the addition of three equivalents of PhMgBr to 2-nitrobiaryls at 0 °C in THF leads to the rapid (15 min) formation of the corresponding NH-carbazoles in good isolated yields. This transformation affords carbazoles and other fused *N*-heterocycles via the TM-free regioselective intramolecular amination of aromatic C(sp²)-H bonds and currently it is the shortest and lowest temperature method known to access these types of compounds most conveniently. Using this approach we have been able to prepare two potent anti-HIV carbazole natural products in just two steps each, on a multi-hundred milligram scale, that allows the rapid evaluation of their unique properties. We were also able to demonstrate that oxygen gas (O₂) in air can be an excellent terminal oxidant in the one-pot TM-free dehydrogenative cross-coupling of nitroarenes with aryl-alkyl and dialkyl ketones. The resulting alpha-arylated ketones were obtained in just 30 minutes at room temperature with substitution patterns that are very difficult and labor-intensive to obtain using other methods. Finally, the benzo[*b*]furan structural motif is widespread in nature, medicines as well as materials, yet current synthetic protocols almost always require the use of TM-catalysts and highly elaborate starting materials to prepare them. We have developed a facile TM-free *O*-arylation of ketone oximes at room temperature using diaryliodonium salts as the arylating agents. Then a protic acid is added and the *in situ* formed *O*-aryl ketone oximes undergo [3,3]-rearrangement/cyclization in the same pot to afford benzo[*b*]furans efficiently.

JAAN LAANE, A-0396, Texas A&M University. MOLECULAR CONFORMATIONS AND VIBRATIONAL POTENTIAL ENERGY SURFACES.

Infrared and Raman spectroscopy have been used to study the potential energy surfaces (PESs), structures, and vibrations of molecules in their electronic ground states while laser-induced fluorescence excitation spectra (FES) of jet-cooled molecules and ultraviolet (uv) absorption spectroscopy were used to investigate electronic excited states. Density functional theory and *ab initio* computations were also carried out to complement the experimental work. The vibrational frequencies and structures of 2,6-difluoropyridine in its S_0 , $S_1(n,\pi^*)$ and $S_2(\pi,\pi^*)$ states were determined. It has a planar structure for S_0 and S_1 but has a barrier to planarity of 256 cm^{-1} for S_2 . The vapor-phase Raman spectra of *cis*- and *trans*-stilbene were recorded and assigned with the help of theoretical calculations. The conformational energetics of the *cis* conformer was analyzed in detail. The FES and uv spectra along with structural computations of benzocyclobutane were analyzed and compared to related bicyclic molecules. The vibrational spectra of 4-silaspiro(3,3)heptanes were analyzed and these show both four-membered rings to be puckered. With the aid of *ab initio* calculations the two-dimensional PES was determined and used to calculate the resulting complex set of quantum energy states and their associated wavefunctions. The far-infrared spectra along with theoretical computations were used to calculate the PESs for four cyclic silanes. These experimentally determined PESs agree remarkably well with the theoretical results. The PESs for 1,3-disilacyclopent-4-ene and 1,3-disilacyclopentane were also determined from their far-infrared spectra and theoretical calculations. The former molecule is planar while the latter has a twisted structure. Current investigations are underway on two bicyclic molecules, 2-cyclopenten-1-one ethylene ketal and 2,4,7-trioxa(3.3.0)octane. Their PESs and their energy levels and wavefunctions will be determined.

KEJILAI, F-1814, The University of Texas at Austin. ELECTRICAL IMAGING OF CHEMICALLY INTERCALATED NANO-MATERIALS.

We are very grateful to the support from the Welch Foundation, which leads to the following exciting progress in the past grant year.

1. Material synthesis and characterization. As the first step of this project, we have obtained high quality 2D materials by both mechanical exfoliation and chemical/physical vapor deposition. Two furnaces were set up in the PI's lab to grow In_2Se_3 , GaSe, MoS_2 , and MoSe_2 on mica or SiO_2/Si substrates. A manuscript based on our electrical mapping of defects on MoS_2 monolayers has been accepted for publication. Two papers on the layer-dependent dielectric constant and photoconductivity in In_2Se_3 are currently in preparation.

2. Chemical intercalation. We have experimented two routes of intercalating metal (copper or lithium) ions into layered chalcogenides or oxides. The first method utilizes tetrakis(acetonitrile)copper(I) hexafluorophosphate in acetone to incorporate Cu into V_2O_5 and MoO_3 . Secondly, MoS_2 samples on Si/SiO_2 were put into the anhydrous tetrahydrofuran (THF) solution of lithium naphthalene in ice-water bath and argon atmosphere. For both processes, the sample thickness increased considerably after the intercalation and the conductivity is much enhanced over the starting materials, as measured by our impedance probe. We are currently optimizing the parameters for better control of the reaction and cleaner sample surface. One manuscript is in preparation to describe the first process and the accompanied insulation-metal transition.

3. Oxidation and aging effect. Broadly speaking, many chemical reactions involving 2D materials, such as oxidation and reduction, are initiated by intercalation from the side surface because of the strong intralayer covalent bonding v weak interlayer van der Waals bonding. Using the impedance imaging technique, we have investigated the real-space thermal oxidation of WSe_2 into WO_3 and electrical aging of black phosphors. Both processes are highly anisotropic and dominated by the diffusion of oxygen or water molecules from the sample edges. We are preparing two high-impact papers on the above topics.

DAVID L. LAMBERT, F-0634, The University of Texas at Austin. THE CHEMICAL COMPOSITION OF STARS.

Atomic and molecular absorption lines in stellar spectra were analyzed to determine elemental and isotopic concentrations in stellar atmospheres and interstellar clouds to test theories about the production and destruction of nuclides by stars, the evolution of stars, and the formation of the Galaxy.

Among this year's projects was an analysis of interstellar CN absorption lines formed in diffuse clouds in front of nearby bright stars. This analysis provided the first determination of the N isotopic ratio $^{14}\text{N}/^{15}\text{N}$ ($= 278 \pm 18$) in diffuse clouds. Recent theoretical studies of ^{15}N synthesis by stars strongly suggest that our novel result can be accounted for only if substantial amounts of ^{15}N are made by novae.

Studies have continued of the composition changes induced in stars as they evolve from H-burning dwarf stars to He-burning giant stars. A detailed study of carbon and nitrogen in stars with masses of around ten solar masses show that giants are C-poor and N-rich relative to their progenitors, as predicted.

ALAN M. LAMBOWITZ, F-1607, The University of Texas at Austin. DNA TARGET SITE RECOGNITION BY MOBILE GROUP II INTRONS.

1) We used directed evolution to select group II introns that function at lower Mg^{2+} concentrations, providing insight into a key Mg^{2+} -dependent conformational change in group II intron RNAs and potentially enabling more efficient targetron function in eukaryotes (Truong et al. 2013). (2) We collaborated with Dr. Andrew Ellington (UT Austin) to develop facile methods for large-scale bacterial genome engineering by using targetrons to position recombinase sites, enabling multiple, large site-specific insertions and deletions in diverse bacterial genomes without selection (Enyeart et al. 2013). (3) We collaborated with the USAF to adapt targetrons for biodefense against the bacterial pathogen *Bacillus anthracis* (Saldanha et al. 2013). (4) With collaborators, we used our newly developed thermotargetron system to analyze the contribution of cellulosome components to cellulose hydrolysis in the thermophilic anaerobic bacterium *Clostridium thermocellum* (Hong et al. 2014). (5) We published a comprehensive review of biotechnological applications of mobile group II introns in gene targeting and as a source of novel thermostable reverse transcriptases, which enable new approaches to next-generation RNA sequencing and the analysis of non-coding RNAs (Enyeart et al. 2014).

CHRISTY F. LANDES, F-1787, Rice University. EXPLOITING MOLECULAR FLUORESCENCE TO PROBE LOCAL CHEMICAL DYNAMICS.

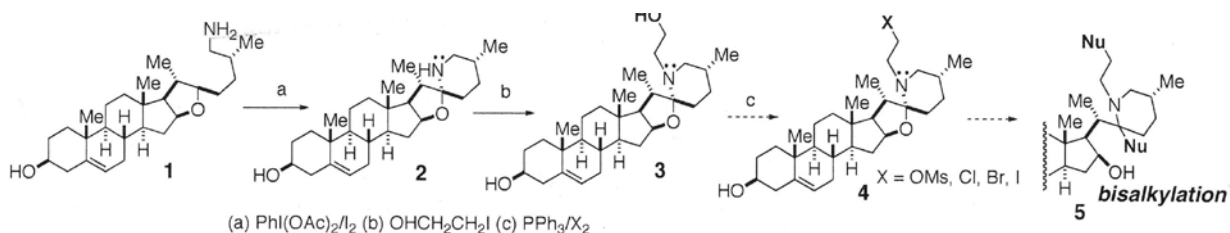
The past year has seen further productivity towards our overall goal to advance single-molecule spectroscopic techniques to understand biomolecular dynamics. We focused on developing new methods to increase information content in the low signal-to-noise data typical of single-molecule measurements, and applying our new methods to acquire quantitative information about an important biomaterials problem, namely protein separations. In one paper, (*ACS Appl. Materials and Interfaces*, 2013, pp 9338-9343), we presented a method by which to break the diffraction limit of optical microscopy using so-called 'super-resolution' analytical techniques, while also extracting equilibrium and non-equilibrium rate constants. Based on our total body of Welch funded work, we were invited to submit a perspective that reviewed the current state of knowledge (*PCCP*, 2014, pp 624-634) including our own contributions on using advanced analysis techniques to track single particles in noisy systems. Most importantly, we applied our extensive data analysis methods to interesting biomaterials problems. We were interested in testing the hypothesis that chromatographic ion-exchange separations involve higher order interactions than 'simple' electrostatics. By applying our experimental and analytical methods, and by relating our experimental results to a theory for adsorptive separations, we demonstrated that ion-exchange adsorptions are indeed based in an underlying geometry, rather than just point-charge interactions. This project has resulted in two papers so far (*PNAS*, 2014, pp 2075-2080; *J. Chromatography A*, 2014, pp 135-142), and we expect more to come as we continue our project. Welch funding was crucial both to our short-term goal of methods development on exploiting molecular fluorescence fluctuations and also to our broader collaborative projects.

OLEG V. LARIONOV, AX-1788, The University of Texas at San Antonio. NEW ENANTIOSELECTIVE STRATEGIES FOR THE SYNTHESIS OF HPI NATURAL PRODUCTS.

In the second year of the research supported by the Welch Foundation we have focused on the study of the mechanism and the synthetic scope of the new catalytic reactions that we discovered in the first year. We have investigated the nature of the catalyst and the details of the catalytic cycle of the inverse-electron demand cycloaddition reaction of nitrosoalkenes. We have also investigated new approaches to construction of the hexahydropyrrolo[2,3-*b*]indole (HPI) core as it relates to our synthetic efforts to HPI natural products. We have developed a one-step synthesis of C3-N-HPI compounds by a reaction of arenediazonium compounds with tryptamines and studied the mechanism of this transformation. We have also developed a new copper-catalyzed reaction of heterocyclic *N*-oxides with Grignard nucleophiles that directly affords 2-substituted *N*-heterocycles. In addition, a C2-selective transformation of *N*-oxides to 2-trifluoromethyl-substituted *N*-heterocycles has been developed, and preliminary mechanistic details have been published. These two methods establish an efficient strategy for highly regioselective synthesis of *N*-heterocycles. We are excited about these discoveries and continue to pursue development of this efficient C-C bond-forming methodology. A new and environmentally benign method of synthesis of *N*-oxides has also been investigated synthetically and mechanistically. Furthermore, an unprecedented palladium-catalyzed 08-selective C-H-functionalization of quinoline *N*-oxides has been discovered. The process will provide new ways of synthesis of structurally challenging *N*-heterocyclic compounds that are functionalized in distal positions other than C2. All in all, the second year has resulted in a highly productive expansion of our initial discoveries, and we are looking forward to accomplishing our research goals in the third year.

SEONGMIN LEE, F-1741, The University of Texas at Austin. DEVELOPING POTENT SOLMARGINE ANALOGS.

During the 2013-2014 funding period, we have made significant progresses in the synthesis of solmargine-based potential bisalkylating agents, which may generate two alkylation sites and alkylate bio-nucleophiles such as DNA and proteins. We have efficiently prepared a key ethanolamine intermediate **3** from alkylamine **1** using our developed novel aminyl radical cyclization method. For the 2014-2015 grant period, we will make latent bisalkylating agent **4** by modifying hydroxyl group in ethanol amine **3**, and will test DNA alkylation activity of compound **4**. If the compound **4** exhibits DNA alkylation activity, we will co-crystallize the alkylated DNA with human DNA polymerases β and η , which are known to play an important role in chemotherapeutics resistance in various cancer cells.



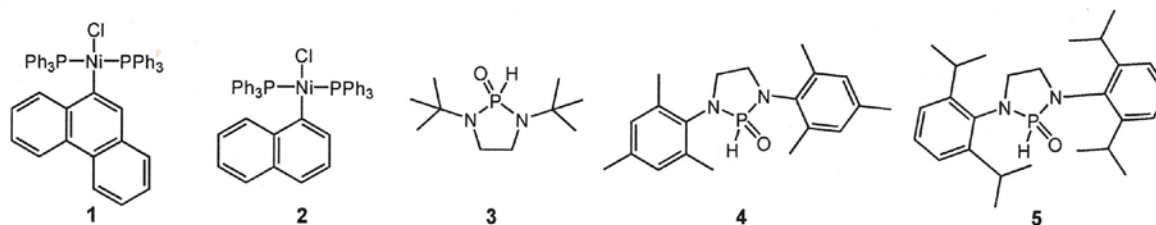
T. RANDALL LEE, E-1320, University of Houston. ALIPHATIC DITHIOCARBOXYLATES, XANTHATES, AND DITHIOCARBAMATES ON METAL SUBSTRATES AND METAL NANOPARTICLES.

We examined the order and coverage of SAMs derived from selected monodentate and bidentate thiol-based adsorbates (Jang et al. *J. Phys. Chem. C* 2013), developing guiding principles for optimal adsorbate design. In related work, we successfully developed a family of custom-designed bidentate

adsorbates having an aromatic-based headgroup for use in the preparation of stable thin films terminated with carboxylic acid moieties (Lee et al. *Langmuir* 2013). In complementary efforts to generate stable nanoscale coatings, we explored two classes of new tridentate adsorbates: one having a headgroup based on Kemp's triacid (Burapol et al. *Langmuir* 2013), and the other utilizing a quaternary carbon as the center of the chelating unit (Tian et al. *Bellstein J. Nanotechnol.* 2014). These studies offered convincing evidence of the importance of chelation for the generation of stable organic thin film coatings on metal surfaces. We also continued to explore the performance of hydrocarbon-based dithiocarboxylates, dithiocarbamates, and particularly xanthates as unique SAM adsorbates and for their utilization as inks for microcontact printing (Moore et al. *Langmuir* 2013). Our studies indicate that, when compared to normal alkanethiol adsorbates, these adsorbates will exhibit enhanced fidelity and thus enhanced patterning efficiency. In separate studies, we reported the preparation of stable SnO₂ thin films doped with homogeneously distributed metal nanoparticles (Lee et al. *Chem. Mater.* 2013 and Lee et al. *Thin Solid Films* 2014). These systems offer important advantages in solar-to-fuel energy conversion. Separate studies in the area of magnetic nanoparticles for biosensing led to a comprehensive review on the relationships between magnetic nanoparticle structure, composition, and properties (Kolhatkar et al. *J. Mol. Sci.* 2013). In additional nanoparticle-related work, we developed a unique polymeric coating for gold nanoparticles that offers fully reversible aggregation and de-aggregation, offering a new and reusable biosensing technology (Park et al. *Coil. Polym. Sci.* 2014).

XIANGYANG LEI, V-1815, Lamar University. NEW NICKEL(II) σ -ARYL COMPLEXES AS CATALYSTS FOR SUZUKI CROSS-COUPLING REACTIONS.

During the first grant year, one postdoctoral fellow (Dr. Feng Hu), one graduate (Ms. Blessy N. Kumpati) and one undergraduate (Mr. Timothy Brown) student worked on the proposed research. We synthesized one new nickel(II) σ -aryl complex (**1**) and investigated its application as precatalyst in the Suzuki cross-coupling reactions of aryl tosylates with arylboronic acids. The results show that complex **1** is an efficient precatalyst and the catalytic system can tolerate a variety of functional groups. These results have been published on *Tetrahedron* in 2014. Meanwhile, we synthesized one known nickel(II) σ -aryl complex (**2**), an analog of complex **1**, and three air- and moisture-stable diaminophosphine oxides (**3-5**). With complexes **1-2** as precatalysts and phosphine oxides **3-5** as preligands, the Suzuki cross-coupling reactions of aryl chlorides with arylboronic acids have been investigated. The results show that diaminophosphine oxides are efficient preligands for the Suzuki cross-coupling reactions of aryl chlorides with arylboronic acids catalyzed by Ni(II) σ -aryl complexes. To our best knowledge, this is the first investigation of diaminophosphine oxides as preligands in the Ni-catalyzed Suzuki cross-coupling reactions. The manuscript based on these results has been submitted to *European Journal of Organic Chemistry* for publication.



BING LI, I-1713, The University of Texas Southwestern Medical Center. BIOCHEMICAL AND FUNCTIONAL ANALYSIS OF HISTONE CLIPPING.

During the past grant period, we continued our effort to identify novel histone clipping enzymes. We purified native NMA111 from cells, which presumably includes all ancillary proteins for its activity. However, we did not detect any significant clipping activity of this native form in our *in vitro* assay, suggesting that histones may not be the substrates for this protease. The chicken homolog of Glutamate De-hydrogenase (Gdh1 and Gdh3) was shown to display histone clipping activity. We therefore purified recombinant forms of these two proteins using baculo virus and bacterial expression systems. Although we have not detected significant cleavage of histones, we found that Gdh3 specifically interacts with histone H3. Interestingly, the histone cleavage activity of nuclear extracts was stimulated by the addition of Gdh3, suggesting that these two proteins may play regulatory roles in histone cleavage, or nuclear extracts contain activating factors for these two enzymes.

Towards our second specific aim, we have mapped the histone cleavage sites in our biochemical system through protein sequencing and mass-spectrometry. Mutations of the residues around the cleavage site have significantly reduced the histone clipping *in vivo*. We are currently testing if these mutations influence expression patterns of those genes where histone clipping was detected upon transcriptional induction in previous studies.

GUIGEN LI, D-1361, Texas Tech University. CHIRAL *N*-PHOSPHONYLIMINES-CONTROLLED ASYMMETRIC REACTIONS OF HALO ENOLATES.

The synthesis and production of pharmaceuticals and chemicals in industrial and academic labs require much use of materials, manpower and energy; and at the same time, generate tons of wastes daily, particularly, the disposal of silica gel wastes and solvents has been imposing significant environmental negative impacts in the world. To avoid or minimize this situation, the new concept of GAP (Group-Assisted Purification) chemistry was established and applied for a series of reactions and productions, particularly, for the synthesis of protected amino acids and peptides. *N, N'*-Di-(1-naphthylmethylene)-1,2-cyclohexyldiamino *N*-phosphonyl protected amino acids, such as L-Pro-OBn, D-Ala-OMe and L-Phe-OMe and L-Tyr, have been

generated and utilized for the synthesis of peptides with biphalin as an example that belongs to opioid pain killers. Due to the GAP protection groups, the products can be purified simply by washing the crude mixtures with inexpensive petroleum solvents or co-solvents without the use of traditional purifications of chromatography, recrystallization, etc. The GAP groups can be cleaved with nearly quantitative recovery of auxiliaries *via* a one-time extraction with *n*-butanol. The GAP-peptide synthesis can overcome shortcoming of the solid-phase-peptide synthesis (SPPS) and the liquid-phase-peptide synthesis (LPPS). The GAP chemistry has also been utilized for the synthesis of an anti-cancer drug, Velcade. At the key step, asymmetric borylation of an imine anchored with a chiral *N*-phosphinyl auxiliary was conducted to give the optically pure isomer (*dr* > 99:1) and good yields. Several new multicomponent domino reactions were investigated under microwave irradiation leading to the formation of a series of heterocycles for organic and medicinal research. Finally, new oxidative dehydrogenative couplings of pyrazol-5-amines for the selective synthesis of azopyrrole derivatives have been developed. The former reaction simultaneously installs N-N and C-I bonds through iodination and oxidation whereas the latter involved a copper-catalyzed oxidative coupling process.

PINGWEI LI, A-1816, Texas A&M University. THE STRUCTURAL BASIS OF MICROBIAL DNA SENSING IN INNATE IMMUNITY.

We have conducted extensive studies of the mechanism of microbial DNA sensing by cGAS during this grant year. First, we have determined the crystal structures of human cGAS catalytic domain in two crystal forms. Second, we have determined the crystal structure of mouse cGAS catalytic domain bound to an 18 bp dsDNA. This structure revealed that cGAS binds to dsDNA through two binding surfaces and DNA binding induced oligomerization of cGAS is needed for its activation. To test this model from our structural studies, we have generated a number of mutants of mouse cGAS and confirmed that DNA binding at both binding sites are needed for the activity of cGAS. We also conducted DNA binding studies of these mutants and observed that mutations at the new binding site we observed in the structural studies are critical for the cooperative dsDNA binding by cGAS. DNA binding induced oligomerization of cGAS was confirmed by small angle X-ray scattering and analytical ultracentrifugation. Third, we have determined the structure of the enzymatic product of cGAS, 2', 5' cGAMP, bound to mouse cGAS and the 18 bp dsDNA. This structure revealed how the product binds to the active site of cGAS before its release from the enzyme. In summary, these structural studies of cGAS and its complex with dsDNA revealed the mechanism of cGAS activation. This work was published in *Immunity*, a prestigious journal in immunology.

XIAOQIN (ELAINE) LI, F-1662, The University of Texas at Austin. SURFACE PLASMON ENHANCED SPECTROSCOPIC RULERS.

We aim to apply this powerful spectroscopic method; surface plasmon enhanced spectroscopic rulers to study properties of metallic and semiconductor nanostructures. These nanostructures can be considered as artificial molecules that consist of coupled quantum dots and metallic nanostructures which can be fabricated and engineered on nanometer scales with precisely tailored properties. By studying these well-controlled model systems, one can learn how to interpret spectra obtained from more complicated nano-systems, bio-molecules, etc. In this grant year, we have published five articles in *Advanced Materials*, *Nature-Communication*, *Physical Review Letters*, *Physical Review B* and *New Journal of Physics*, respectively. Another article has been accepted at *Advanced Materials*. These six papers focus on fabrication and characterization of metallic and semiconductor nanostructures. Another article on bio-sensing is currently under review at *Nature-Photonics*.

ROGER L. LICHTI, D-1321, Texas Tech University. ENERGIES AND DEFECT CHEMISTRY FOR MUONIUM IN OXIDE SEMICONDUCTORS.

We find that muonium (Mu) forms a shallow donor state in all transparent conducting oxides (TCOs) investigated to date, which implies that hydrogen will contribute to the prevailing n-type conductivity in this class of oxides. Muon spin depolarization in zero applied field shows that Mu^+ becomes diffusively mobile near 300K in In_2O_3 with a thermal barrier of 0.43 eV and quickly traps at another impurity, forming a Mu-Defect pair which has a dissociation energy of 0.91 eV. We are currently modeling the trap-and-release dynamics that govern high-temperature diffusion in an effort to extract the trapping and release rates as a function of temperature directly from the time-dependent polarization data. In HfO_2 , a high-K dielectric that is replacing SiO_2 as an FET gate oxide, an implanted muon forms a short-lived intermediate Mu^0 state prior to reaching its O-Mu bonded ground state. In TiO_2 , MuSR spectra confirm that the neutral Mu^0 has its electron localized on a nearby Ti ion (as Ti^{3+}) rather than forming an effective mass shallow donor as in the other TCO compounds. This structure was also found for H^\bullet in TiO_2 by EPR, adding to the growing inventory of systems where H and Mu show identical structures. Our data on the low-temperature semiconducting phase of VO_2 shows anti-ferromagnetic order below 35K in the first demonstration of AF magnetism in this compound. T_N increases significantly when VO_2 is doped to disrupt the V^{4+} - V^{4+} dimerization characteristic of the low-T phase. These results indicate that spin-zero dimer formation and the competing long-range AF order are very delicately balanced in VO_2 .

PAUL A. LINDAHL, A-1170, Texas A&M University. CHARACTERIZATION OF LOW-MOLECULAR-MASS IRON AND MANGANESE COMPLEXES IN EUKARYOTIC CELLS.

We made significant progress towards our objectives last year, publishing four papers with the support of the Welch Foundation. Each study focused on aspects of iron trafficking in human or yeast cells. In the first study (Jhurry *et al.*, 2013) we characterized the iron trafficking pathways in human (Jurkat) cells, and developed the first mathematical model to describe these pathways. We quantified the major types of Fe in these human cells, including ferritin, mitochondrial Fe, ferric nanoparticles and nonheme high-spin Fe^{II} which probably represents the LMM labile Fe pool. We found that the distribution of Fe in cells grown on transferrin-bound iron differed from that grown on ferric citrate. The mathematical model, which included regulation and cytosolic Fe, was the first to mimic the observed Fe content of these cells grown on different media. The extent of Fe loading into ferritin was less than expected, as was the extent of ROS damage with the formation of nanoparticles. The model reproduced the effect of deleting frataxin, the lack of which causes Friedrich's ataxia in

humans. In the second study (Park *et al.* 2013), we discovered that yeast cells overload with iron when grown past the exponential growth phase. In contrast, the Fe concentration in exponentially growing cells was well regulated. During post-exponential growth, the rate of Fe import exceeds the rate of cell growth, causing a massive accumulation of Fe, mostly in the form of ferric nanoparticles. The extent of ROS damage was again not proportional to the extent of nanoparticle formation. A mathematical model was developed to explain the Fe accumulation mechanism. The model captured the essential trafficking behavior, demonstrating that cells misregulate Fe import when nanoparticles accumulate. The lack of regulation for Fe is possibly unique in cell biology, due to the unique chemistry associated with Fe nanoparticle formation. In the third study (Park *et al.* 2014); we studied the iron content in yeast cells that were deficient in adenine. Such cells generate a toxic adenine precursor that is sent to vacuoles via a glutathione conjugate. Vacuoles are the site of Fe storage in yeast cells; normally Fe is found in vacuoles as mononuclear high-spin Fe^{III} with a small quantity of Fe^{III} nanoparticles. In this study, we discovered that vacuolar Fe is reduced to the Fe^{II} state as a result of adenine-deficiency. Two Fe^{II} species were detected. One has ligands with predominately N/O donors; the other Fe^{II} species includes some sulfur coordination. Thus, we discovered that vacuolar Fe is redox-sensitive. Increasing the concentration of amino acids and nucleotide bases in the media converted virtually all vacuolar Fe into mononuclear high-spin Fe^{III}, with insignificant amounts of nanoparticles. Glucose levels and rapamycin (which affects the TOR system) affected cellular Fe content as well. This study demonstrates the sensitivity of cellular Fe to changes in metabolism, redox state and pH. In the final study (Cockrell *et al.*, 2014) we examined the iron content of two strains of yeast, namely Δ ccc1 and CCC1-up. Ccc1p is a vacuolar membrane protein that transports Fe and Mn from the cytosol to the vacuole. In this study, we examined the trafficking of these transition metals in these strains which were expected to perturb traffic flow. We used an integrated biophysical approach, centered on Mössbauer spectroscopy, to evaluate the Fe content in these cells. We also developed a mathematical/chemical model to explain the observed strain-dependent changes. A large quantity of nonheme high-spin Fe^{II} was observed, but our model showed that most of it was not used in regulating Fe import into the cell. Most of these Fe^{II} ions probably result from more reduced conditions of the vacuoles in these strains. These are the first models to include cytosolic Fe^{II}, which probably constitutes the LMM pool.

STEPHAN LINK, C-1664, Rice University. CHEMISTRY MEETS SURFACE PLASMONS.

We investigated the electron transfer between Au nanorods and graphene using single particle spectroscopy to access the homogeneous linewidth free from ensemble-averaged broadening. We assigned the damping of the surface plasmon resonance for nanorods on graphene compared to nanorods on quartz to charge transfer between plasmon generated hot electrons and graphene. Detailed analysis of the plasmon linewidth coupled with electromagnetic simulations yielded an electron transfer time of 160 ± 30 fs and a 10% efficiency. Furthermore, changes in the plasmon linewidth and resonance energy of Au nanospheres were induced in an electrochemical cell, allowing us to follow nanoparticle charging dynamically with the potential to probe in the future (photo)catalytic redox reactions on the nanoparticle surface. Such photo-induced surface chemistry requires the production of hot electrons through nonradiative plasmon decay. We found that an admixture of Co in hollow Au nanoshells can strongly enhance hot electron generation. In addition, we studied plasmon damping in nanoparticle dimers using an electrostatic model, achieved optical gain of surface plasmons in Au nanowires through coupling to organic dye molecules, characterized energy propagation around a 90° turn in a nanoparticle chain, and quantified the contributions from radiative and nonradiative decay of surface plasmons in Au nanowires with different cross sections. In work still under review, we studied the effects of near-field and far-field plasmon coupling on the optical properties of Au and Al nanoparticle arrays and investigated the surface enhanced Raman scattering of 4-mercaptobenzoic acid bound to spiky Au nanoshells. Finally, we wrote a tutorial review article on current single particle spectroscopy techniques.

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

During this grant year, we applied MAPPER, the ER-PM junction marker, to study the regulation and functions of ER-PM junctions. We demonstrated that ER-PM junctions are dynamically regulated by extended synaptotagmin-1 (E-Syt1), an ER membrane protein that translocates to ER-PM junctions upon increases in cytosolic Ca²⁺. We further found that this dynamic regulation is important for the recruitment of Nir2, a phosphatidylinositol (PI) transfer protein, to ER-PM junctions and for the regeneration of PI 4,5-bisphosphate (PIP₂) at the PM following receptor-induced hydrolysis. These results uncovered a feedback mechanism that replenishes PM PIP₂ during receptor-induced Ca²⁺ signaling via the Ca²⁺ effector E-Syt1 and the P1TP Nir2 at ER-PM junctions and were published in a paper in *Cell Reports* in November 2013.

In addition, we generated a new imaging probe for visualizing ER-PM junctions using photo-activated localization microscopy (PALM). By performing super-resolution imaging, we found that the size and shape of ER-PM junctions are strikingly uniform and remain the same during receptor-induced Ca²⁺ signaling. These results provide the first en face measurements of ER-PM junctions and suggest the existence of mechanisms defining the shape and size of ER-PM junctions.

Lastly, we developed mCherry-MAPPER-GCaMP for monitoring Ca²⁺ signaling at single ER-PM junctions where store-operated Ca²⁺ (SOC) influx occurs. This new probe successfully eliminated the strong cytosolic background caused by FKBP-R-GECO1 developed in the previous grant year and will be applied to measure local SOC influx at subcellular regions during physiological processes, such as cell polarization and migration.

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

Formycin Biosynthesis. A formycin biosynthetic pathway has been proposed based on our genomic sequencing results of *S. kaniharaensis*. Our initial efforts have been directed at investigating the Pur homologues, PurC, PurB, PurH, and PurA. These enzymes are hypothesized to be responsible for the later steps in formycin biosynthesis due to their similarity to AMP biosynthetic enzymes (Purs) in *E. coli*. The proposed substrate of PurC in the formycin

pathway has been chemically synthesized. While this compound is a substrate for *E. coli* PurC, it cannot be processed by *S. kaniharaensis* PurC. It is not clear whether the negative result is due to the inactivity of the purified enzyme or incorrect assignment of the proposed pathway. We are now preparing a putative downstream intermediate as a possible substrate for *S. kaniharaensis* PurH. Results with this compound and PurH will help to support or refute the proposed pathway.

Nogalamycin Biosynthesis. The D-ring of the C1-hydroxylated nogalamycin aglycone is connected to nogalamine via an *O*-glycosidic bond at C1 and a *C*-glycosyl bond at C2. Our aim is to elucidate the mechanisms of modification and glycosylation that result in the coupling of nogalamine to this anthracycline aglycone core. This coupling results in the introduction of an atypical epoxyoxocin ring to the core structure. We have recently reconstituted the biosynthetic pathway for TDP-nogalamine using purified enzymes *in vitro*. Because few C1-hydroxylated anthracyclines have been reported and the nogalamycin aglycone is not readily accessible, we originally proposed to bioengineer daunomycin producing *S. peucetius* to hydroxylate daunomycin *in vivo* as an analog for the nogalamycin aglycone. Instead, we have now developed an efficient scheme to chemically synthesize the nogalamycin aglycone directly. The synthesis is nearly complete. Once it is finished, we will carry out incubations of the aglycone and TDP-nogalamine with the enzymes of interest (i.e., SnoO and SnoK) to investigate formation of the epoxyoxocin ring.

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.

Bacterial type III secretion machines are widely used to inject virulence proteins into eukaryotic host cells. These machines are evolutionarily related to bacterial flagella and consist of a large cytoplasmic complex, a transmembrane basal body, and an extracellular needle. The cytoplasmic complex forms a sorting platform essential for effector selection and needle assembly, but remains largely uncharacterized. In this grant year, we used high throughput cryo-electron tomography to visualize intact machines in a virulent *Shigella flexneri* strain, genetically modified to produce tiny minicells. A 3.4 nm resolution *in situ* structure of the intact machine determined by sub-tomogram averaging reveals the cytoplasmic sorting platform for the first time. This platform consists of a central hub and six spokes, with a pod-like structure at the terminus of each spoke. Molecular modeling of wild-type and mutant machines allowed us to propose a pseudo atomic model of the sorting platform, in which the hub consists mainly of a hexamer of the Spa47 ATPase, while the MxiN protein comprises the spokes and the Spa33 protein forms the pods. Multiple contacts among those components are essential to align the Spa47 ATPase with the central channel of the MxiA export gate and form a unique tandem nanomachine. The molecular architecture of the *Shigella* type III secretion machine and its sorting platform provide the structural basis for dissecting the mechanisms underlying type III secretion and pathogenesis, and also highlight the major structural distinctions from bacterial flagella.

QINGHUA LIU, I-1608, The University of Texas Southwestern Medical Center. MECHANISTIC STUDIES OF THE *DROSOPHILA* RNA INTERFERENCE PATHWAY.

The catalytic engine of RNA interference (RNAi) is the RNA-induced silencing complex (RISC), wherein single-strand siRNA guides Argonaute 2 (Ago2) endoRNase to catalyze sequence-specific mRNA cleavage. We previously reconstituted *Drosophila* core RISC using recombinant Dicer2-R2D2 and Ago2 proteins, and used this system to identify C3PO, an octameric complex of six Translin and two Trax, as a novel endoRNase that promotes fly and human RISC activation. We determined the crystal structure of human (h) C3PO (3.0Å) and a 18Å cryoEM structure of C3PO/ssRNA complex using a newly developed ChemiC-Grid EM technology. This innovative method (NIH Eureka Award) allows for selective enrichment and cryoEM imaging of homogenous C3PO/ssRNA complex on the siRNA-conjugated ChemiC films. Our structural and biochemical studies suggest that C3PO has an unprecedented dynamic cycle of catalysis: C3PO exists in different oligomeric states: inactive dimer/tetramer and active octamer. The presence of ssRNA nucleates the assembly of catalytic active octamer, whereas ssRNA cleavage allows C3PO to disassembly into inactive dimer/tetramer. Additionally, the EM structure of C3PO/RNA complex reveals a possible active conformation, where ssRNA is sandwiched between two catalytic Trax subunits on the surface of C3PO octamer. Our studies suggest C3PO has a dynamic catalytic mechanism that is unlike any known nucleases.

WENSHE LIU, A-1715, Texas A&M University. BIOSENSORS FOR SMALL MOLECULES AND ENZYMES.

Fluorescently labeled protein and small molecule entities are sensitive tools to monitor small molecules and enzyme activities. To synthesize fluorescently labeled ubiquitin molecules that can be used as activity sensors of deubiquitinases, we invented a simple approach to functionalize the ubiquitin C-terminal carboxylate. A paper described this progress was published in *ChemBioChem*. Previously we showed that a pyrrolysyl-tRNA synthetase (PylRS) mutant together with its amber suppressing tRNA^{Pyl} was able to incorporate more than 20 para- and meta-substituted phenylalanine derivatives. We extended this discovery to reveal that this same enzyme-tRNA pair can mediate the incorporation of several ortho-substituted phenylalanine derivatives and phenylalanine analogs with large substituents at meta and para sites. These genetically encoded noncanonical amino acids contain a large variety of functionalities including azide, alkyne, ketone, alkene, and aldehyde and therefore enable multiple methods to fluorescently label proteins. Three papers describing these progresses were published in *ACS Chemical Biology* and *Chemical Communications*. We also investigated the mechanism of 1,2-dipolar nitrilimine-alkene cycloaddition for fluorescently turn-on labeling proteins incorporated with *N*^ε-acryloyl-lysine and revealed that this reaction is ultra-fast. A paper describing this progress is published in *Chemical Communications*. Another breakthrough we made in the past year was to demonstrate the rare AGG codon in *E. coli* could be successfully reengineered to code noncanonical amino acids. A paper describing this progress has been published as an ASAP article in *ChemBioChem*.

XIN LIU, I-1790, The University of Texas Southwestern Medical Center. STRUCTURAL AND BIOCHEMICAL STUDIES OF GENE REPRESSION BY POLYCOMB REPRESSIVE COMPLEX 2: CATALYSIS AND RECRUITMENT.

We have made the following major achievements toward the research objective in the past year.

1. After 2-year trials we have successfully reconstituted an active 150KDa PRC2 ternary complex by yeast fermentation. All previous biochemical work of PRC2 was based on the insect cell expression system, the turnaround time of which is much longer than yeast fermentation. Indeed, using our unique yeast expression method we have made and tested more than thirty versions of the PRC2 complex in the past year to screen for crystallization conditions and carry out biochemical assays. Manuscript is in preparation to describe this novel expression system for PRC2 function studies. 2. Previous work suggested that human PRC2 forms a dimer *in vivo* and *in vitro*, although the molecular basis is unclear. We have discovered a molecular determinant for PRC2 dimerization by screening mutations and truncations for diminished oligomerization. We have also characterized the PRC2 dimer by size exclusion chromatography, analytical ultracentrifugation, photocrosslinking, and electron microscopy (in collaboration with Junjie Zhang's lab at Texas A&M University), from which we are now deriving a molecular architecture of the PRC2 dimer. 3. ncRNA binding is a key aspect of PRC2 regulation, in particular PRC2 recruitment to chromatin. We have characterized the ncRNA binding affinity and specificity of PRC2 by *in vitro* EMSA assay and found that our minimal active PRC2 complex displays a high selectivity toward sense HOTAIR ncRNA against its anti-sense counterpart, which differs from the ncRNA binding behavior of the PRC2 holo-complex. We have come up with a hypothetical model to explain the observed data, which we believe suggests a new layer of regulation mechanisms for PRC2 functions *in vivo*. Overall, we have made significant progress toward the research objective in the past year. We are currently preparing manuscripts and expect to publish two to three original papers in the next fiscal year.

YI LIU, I-1560, The University of Texas Southwestern Medical Center. BIOCHEMICAL MECHANISMS OF SMALL RNA PRODUCTION PATHWAYS.

Significant portions of eukaryotic small RNA are produced from repetitive DNA loci in fungi to animals. How small RNAs are specifically produced from repetitive DNA loci is not clear. Quelling is an RNAi-related phenomenon that post-transcriptionally silences repetitive DNA in *Neurospora*. We previously identified a type of DNA damage-induced small RNA called qiRNAs that originate from the repetitive ribosomal DNA. To understand how small RNAs are generated from repetitive DNA, we carried out a genetic screen to identify genes required for qiRNA biogenesis. We discovered that a factor directly involved in chromatin remodeling and homologous recombination is essential for qiRNA production. In addition, we discovered that convergent transcription induces a new type of DNA methylation that is mediated by small non-coding RNA, uncovering a previous unexpected role for small RNA in chromatin modifications. Together, our results uncovered two distinct mechanisms in small RNA production and function.

In addition to these studies, we have another study that discovered a novel mechanism for which antisense RNA that triggers gene silencing and is required for circadian clock function. This study established long non-coding RNAs as essential factors in the gene regulatory network of circadian clocks.

STEVE W. LOCKLESS, A-1742, Texas A&M University. THE STRUCTURAL BASIS FOR LIPID REGULATION OF MEMBRANE PROTEIN FUNCTION.

We made progress on three fronts this past year. First, we have measured the inherent ion-binding properties of a variety of channels that selectively transport K^+ ions, Na^+ ions or have no preference. To our surprise, the channels with no transport preference have a strong affinity for K^+ ions over Na^+ ions at equilibrium. This demonstrated for the first time that the equilibrium ion-binding properties of channels do not correlate with their selective ion conduction. We propose a model for selective ion conduction that requires both the equilibrium preference as well as the number of ions bound within the channel. We will now test how changing the lipid environment alters the selectivity and number of ion bound to a channel.

Second, we have determined conditions to remove tightly bound lipids from KcsA without denaturing the protein. These de-lipidated channels were used to obtain crystals that diffract to $\sim 3\text{\AA}$. We will now optimize conditions to obtain higher resolution data to ask how altering the molecules bound to the lipid-binding sites change the distribution of ions in the selectivity filter.

Third, we examined how lipophilic isoprenyl groups interact with a class of membrane enzymes called UbiA. UbiA can be obtained in high quantities and we measured binding of various isoprenyl molecules to the enzyme. Now we will examine the specificity determinants of this lipid-enzyme interaction.

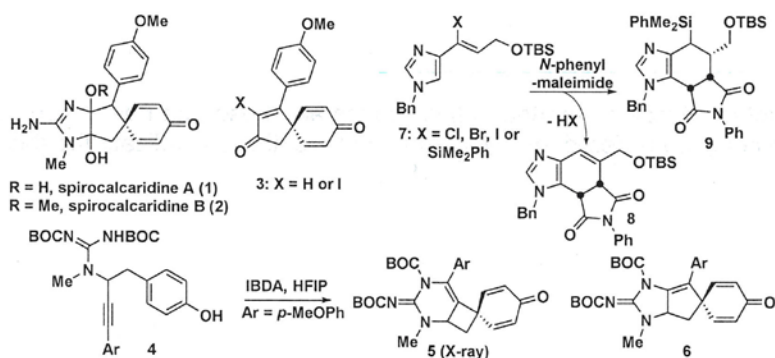
JUN LOU, C-1716, Rice University. DEVELOPMENT OF NANOMATERIALS FOR LOW COST SOLAR ENERGY HARVESTING.

In this grant year, we have largely focused on developing 2D materials and its possible applications in solar energy harvesting and other optoelectronic/electronic devices. In general, the growing interest in understanding the unique physics of two dimensionally confined layered materials has motivated the research of their growth process and its chemical modifications. Molybdenum disulfide (MoS_2) is a member of this group of atomic layers which has been extensively studied by my group for its unique monolayer characteristics. A novel MoS_2 transparent counter electrode for dye-sensitized solar cells was investigated. In order to enhance the catalytic activity of the electrode, active edge sites are created artificially by patterning holes on MoS_2 atomic layers. Electrochemical analysis shows that the electrochemical activity is significantly improved after the patterning of holes. The photon-to-electron efficiency of the dye-sensitized solar cells based on MoS_2 atomic layer counter electrodes is increased remarkably from 2% to 5.8% after the hole patterning. Additionally, MoS_2 single layers have shown considerable tunability in many of their physical properties that show great promise in future electronic and optoelectronics. We carefully investigated the exfoliation process, direct sulfurization, and chemical vapour deposition of MoS_2 monolayers as major approaches in preparation

of these atomic layers. We reveal the predominant types of point and grain boundary defects in the crystal structure of polycrystalline MoS₂ using transmission electron and examine the general electronic properties of single crystalline MoS₂ and study the role of grain.

CARL J. LOVELY, Y-1362, The University of Texas at Arlington. TOTAL SYNTHESIS OF IMIDAZOLE-CONTAINING NATURAL PRODUCTS.

Much of the focus of this year's activities has been directed towards solving critical issues to advance total synthesis efforts. For example, we are actively pursuing tactics for the construction of the spirocyclic framework found in the *Leucetta* alkaloids spirocalcaridine A (**1**) and B (**2**). We have prepared and investigated the elaboration of two spiro dienone systems **3** that while yielding promising results have now evolved in the tandem-sequence from the propargylamine **4**. Whereas in this initial set of experiments the 4,6-fused ring system **5** is formed in preference to the required 5,5-system **6**, we are actively exploring this transformation in order to redirect it through the desired manifold and to improve the efficiency. In the context of several targets in the oroidin family we have begun to explore the utility of heterosubstituted vinylimidazoles **7** in Diels-Alder reactions. We have found that halo-substituted systems engage in the cycloaddition but undergo subsequent dehydrohalogenation (**7**→**8**) whereas the silyl-substituted systems provide the required substituted cycloadduct (**7**→**9**). We are now evaluating these new dienes in intramolecular Diels-Alder reactions and their subsequent elaboration.



VASSILIY LUBCHENKO, E-1765, University of Houston. NEW TYPE OF ELECTRONIC STATES IN VITREOUS CHALCOGENIDES AND PNICTIDES.

1) We have computed, for the first time, the barrier for activated transport in supercooled liquids without using adjustable parameters. The input parameters are measurable configurational entropy, structure factor and elastic constants. We have thus predicted, for the first time, the glass transition temperature for actual materials. These results can be used to predict the glass-forming ability of actual substances.

2) We have developed a unified thermodynamic-kinetic description for a novel aggregation phenomenon. The aggregates are reversible and are stabilized by transient complexes formed by the solute. The size is determined by the decay kinetics of the complexes, among other things. This discovered mechanism is the probable cause of the puzzling mesoscopic clusters found in protein solutions, which are crucial for nucleation of solid aggregates, both beneficial and harmful.

3) We have established the microscopic cause for the puzzling symmetry breaking that takes place in trimeric near-linear motifs in hypervalently bonded compounds. We have used these results to establish, for the first time, an intrinsic connection between metallic, hypervalent, covalent, secondary, and ionic bonding in solids, which will be the basis for the structure prediction methodology for inorganic compounds, both glassy and crystalline, proposed for the following funding period.

4) We have developed, for the first time, a theory of elasticity for equilibrated amorphous materials, which will be used to simulate the activated dynamics using a radically new methodology. We have determined the elastic constants of such amorphous materials self-consistently.

ROBERT R. LUCHESE, A-1020, Texas A&M University. REACTION DYNAMICS PROBED BY MOLECULAR-FRAME PHOTOIONIZATION.

The multi-photon dissociative ionization NO₂ has been studied. The results of an experiment that used 400 nm laser pulses of duration 70 fs leading to dissociative ionization were considered. In the experiment, the ejected photoelectron was measured in coincidence with one of the ion fragments produced in the process. Assuming an $n+1$ type excitation process where n photons are absorbed in bound-to-bound transitions and one additional photon is absorbed to ionize the molecule, expressions for the recoil frame photoelectron angular distributions (RFPADs) were developed. Computed RFPADs were compared with experimental data leading to insights into the dynamics of this process. The laser pulses were long enough so that significant changes in geometry could occur during the ionization process. The experimental data for the five photon dissociative ionization process was best described by an initial three-photon excitation to a Rydberg state, followed by bending of the system, then a one-photon ionization step leading to the ground state of the ion. The fifth photon then excited the ion to a dissociative state. General agreement with the experimental data was found for the computed photoelectron kinetic energy, photo-fragment ion

distribution, and RFPADs, although a quantitative agreement has yet to be achieved. Further calculations including more electron correlation effects and additional molecular geometries will be pursued in the future.

LAWRENCE LUM, I-1665, The University of Texas Southwestern Medical Center. MODULATION OF CANONICAL Wnt PATHWAY ACTIVITY USING SMALL MOLECULES.

In the last funding period, we have: a) used a diverse collection of novel Tnks inhibitors to evaluate the effectiveness of targeting Tnks as a means of achieving telomeric shortening in cancerous cells, b) defined a novel chemical capable of directly targeting transcriptional effectors of Wnt-mediated signaling, and c) progressed our studies focused on targeting Wnt signaling in AML. We further discuss here the first two advances. Using a biochemical assay of Tnks function, we re-evaluated a collection of Wnt pathway inhibitors with unknown mechanisms of action previously identified by my group (the IWR compound collection, ~60 compounds). Novel Tnks inhibitors identified by this approach were then subgrouped based on crystallography-based evidence of their mode of attack. From this exercise, we identified a novel approach to drugging poly-ADP polymerases (PARPs) premised upon targeting the adenosine-binding pocket. Typical PARP inhibitors bind the nicotinamide-binding pocket. Given the Trf1 telomere lengthening suppressor is a Tnks substrate, we used this chemical toolkit to test the potential of Tnks inhibitors for inducing telomere shortening. Exposure of cancerous cells to Tnks inhibitors not only induced a DNA damage response at telomeres but also telomeric shortening. These observations are timely given that Imetelstat, an oligo-nucleotide based chemical targeting telomerase, recently faltered in clinical testing due to off-targeting-associated toxicities. Using epistasis-type mapping of additional IWR collection members, we have also identified a novel small molecule (IWR-16) that directly targets the Wnt pathway transcriptional machinery. IWR-16 alters the abundance of phosphorylated and sumoylated proteins including the TCF/LEF transcriptional regulators. Based on this mechanistic framework, we are now pursuing studies aimed at identifying the target of IWR-16 and evaluating its promise as an anti-colorectal cancer agent.

JODIE L. LUTKENHAUS, A-1766, Texas A&M University. TEMPLATE-SYNTHESIS AND SOLUTION-ASSEMBLY OF POLYANILINE FOR ORGANIC ENERGY STORAGE.

In the last grant year, we have completed and published work on Objective 2, redefined Objective 3, and initiated new work on a new class of electroactive polymers. In Research Objective 2, template-synthesized polyaniline:polyacid was incorporated into LbL assemblies, where the electrochemical stability was retained (*ACS Applied Materials & Interfaces* 2013). Given challenges in executing Objective 3, we have redefined the Objective towards incorporating polyaniline:polyacid into hybrid electrodes with reduced graphene oxide. We are preparing two publications describing the LbL assembly of polyaniline:polyacid electrodes via dip and spray and the electrochemical characteristics of these electrodes. Our current, ongoing work in this Objective entails the synthesis of polyaniline/graphene flexible paper electrodes. The polyaniline:polyacid electrode led us to investigate other systems that might possess very high doping levels and stability at highly oxidizing potentials, thus leading to our report on poly(dithienopyrrole)s, which can achieve doping levels of 0.9 - considered to be very high (*Macromolecules* 2014). One review paper was published (*ACS Macro Letters* 2013), and remains a top-downloaded article. This work has involved one post-doc, one graduate student, and one undergraduate student, where only the post-doc was directly supported.

IGOR LYUKSYUTOV, A-1688, Texas A&M University. CHEMICAL DYNAMICS OF COLD/ULTRACOLD MOLECULES AND ATOMIC HYDROGEN.

a) We have achieved reliable operation of the totally redesigned gas input system near room temperature. This has markedly improved the beam quality, especially at low beam speeds. We have also developed and calibrated the Fast Ion Gage based system for measuring molecular beam density. Thereby we have measured beam densities that are markedly higher than previously attained: up to 100 times higher than achieved in a comparable counter rotating supersonic source in Freiburg University, Germany, and up to 10000 times higher than obtained by the Stark decelerator technique. Prospects appear good for obtaining a further beam density increase.

b) We have systematically studied the steps for CVD graphene sensors fabrication including Dirac point shift under the influence of adsorbed gases.

c) We have continued to fabricate and study magnetic properties of the novel magnetic nanostructures with one and two-dimensional periodicities for manipulating and trapping molecular beams.

JIANPENG MA, Q-1512, Baylor College of Medicine. BIOCHEMICAL STUDY OF THE FUSOGENIC CONFORMATIONAL TRANSITION OF INFLUENZA HEMAGGLUTININ.

Influenza virus HA, a homotrimeric glycoprotein crucial for membrane fusion, undergoes a large-scale structural rearrangement during viral invasion. X-ray crystallography has shown that the pre- and post-fusion configurations of HA₂, the membrane fusion subunit of HA, have disparate secondary, tertiary, and quaternary structures, where some regions are displaced by more than 100 Å. To explore structural dynamics during the conformational transition, in this past year, we studied simulations of a minimally frustrated model based on energy landscape theory. The model combines structural information from both the pre- and post-fusion crystallographic configurations of HA₂. Rather than a downhill drive toward formation of the central coiled-coil, we discovered an order-disorder transition early in the conformational change as the mechanism for the release of the fusion peptides from their burial sites in the pre-fusion crystal structure. This disorder quickly leads to a novel metastable intermediate with a broken threefold symmetry. Finally, kinetic competition between the formation of the extended coiled-coil and C-terminal melting results in two routes from this intermediate to the post-fusion structure. Our study reiterates the roles that cracking and disorder can play in functional molecular motions, in contrast to the downhill mechanical interpretations of the "spring-loaded" model proposed for the HA₂ conformational transition.

ALLAN H. MACDONALD, F-1473, The University of Texas at Austin. ELECTRONIC PROPERTIES OF GRAPHENE.

My Welch grant supports theoretical research that is directed toward advancing understanding of the electronic properties of graphene sheets and other two-dimensional materials and ferromagnetic and antiferromagnetic metals. I continue to work on the fundamental properties of atomically two-dimensional graphene and of two-dimensional electron layers at oxide surfaces and interfaces. An important new element of the physical properties of two-dimensional materials is related to the appearance of moire patterns when two-dimensional materials, with different orientations or with different lattice constants are overlaid. We have published a paper that will, I hope, become a landmark in this field. This work develops very general techniques that can be used to predict electrical and optical properties. A new topic which has been added to my Welch program in the past couple of years is the study of topological insulators, materials which have always have two-dimensional surface states that are required to unknot twists in the bulk electronic structure. One of the highlights of the past year is theoretical work that has demonstrated the possibility of achieving photonic topological insulator states in meta-materials. I continue to work with Welch support with superconductivity, bilayer-exciton condensation, and magnetic metal spintronics. I seek phenomena that are both fundamental from a theoretical point of view and have to potential to yield new technology.

FREDERICK M. MACDONNELL, Y-1301, The University of Texas at Arlington. PROTON-COUPLED ELECTRON TRANSFER MECHANISMS OF DNA CLEAVAGE BY PHOTOEXCITED AND GROUND-STATE RUTHENIUM POLYPYRIDYL COMPLEXES.

Visible light irradiation of $[(\text{phen})_2\text{Ru}(\text{phendione})]^{2+}$ ($\mathbf{1}^{2+}$), where phendione = 1,10-phenanthroline-5,6-dione, leads to DNA cleavage in an oxygen independent manner. A combination of NMR analyses, transient absorption spectroscopy, and fluorescence measurements in water and acetonitrile reveal that complex $\mathbf{1}^{2+}$ must be hydrated at the quinone functionality, giving $[(\text{phen})_2\text{Ru}(\text{phenH}_2\text{O})]^{2+}$ ($\mathbf{1H}_2\mathbf{O}^{2+}$), where phenH₂O = 1,10-phenanthroline-5-one-6-diol, in order to access a long lived ${}^3\text{MLCT}_{\text{hydrate}}$ state ($\tau \sim 360$ ns in H₂O) which is responsible for DNA cleavage. In effect, hydration at one of the carbonyl functions effectively eliminates the low-energy ${}^3\text{MLCT}_{\text{SQ}}$ state (Ru^{III} phen-semiquinone radical anion) as the predominant non-radiative decay pathway. This ${}^3\text{MLCT}_{\text{SQ}}$ state is very short-lived (< 1 ns) as expected from the energy gap law for non-radiative decay, and too short-lived to be the photoactive species. The resulting excited state in $\mathbf{1H}_2\mathbf{O}^{2+}$ has photophysical properties similar to the ${}^3\text{MLCT}$ state in $[\text{Ru}(\text{phen})_3]^{2+}$ with the added functionality of basic sites at the ligand periphery. Whereas $[\text{Ru}(\text{phen})_3]^{2+}$ does not show direct DNA cleavage, the deprotonated form of $\mathbf{1H}_2\mathbf{O}^{2+}$ does via a proton-coupled electron transfer (PCET) mechanism where the peripheral basic oxygen sites act as the proton acceptor. Analysis of the small molecule by-products of DNA scission supports the conclusion that cleavage occurs via H-atom abstraction from the sugar moieties, consistent with a PCET mechanism. Complex $\mathbf{1}^{2+}$ is a rare example of a ruthenium complex which 'turns on' both reactivity and luminescence upon switching to a hydrated state.

JOHN B. MACMILLAN, I-1689, The University of Texas Southwestern Medical Center. NEW METHODOLOGY FOR THE DETERMINATION OF ABSOLUTE STEREOCHEMISTRY.

We have continued to develop and expand on our NMR based methodologies for determination of relative configuration. We have utilized our hyphenated MDEC methodologies to aid in the structural elucidation of five new families of natural products. These techniques are critical for resolving difficult stereochemical and spectral overlap issues. The initial driving force for this work was the cytotoxic natural product nigricanoside which we have recently completed the total synthesis of in collaboration with Joseph Ready. The other area we have pursued this year and is the new direction of the Welch grant, is the use of NMR active isotope labels for the discovery of non-enzymatic biosynthetic reactions, such as those used in the biosynthesis of the ammosamides and the discoipyrroles. We have been able to exploit a combination of ¹⁵N and ¹³C NMR probes to look for incorporation into natural product frameworks. In the case of the discoipyrroles we have monitored the entire non-enzymatic biosynthesis pathway through the use of ¹⁵N-anthranilic acid and ¹³C labeled benzaldehyde coupled with 1- and 2-D NMR.

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

A new computer simulation method was developed to track evolution of critical points (minima and saddles) on a molecular potential energy surface as a function of the applied mechanical stress. In addition to providing a computational advantage by avoiding saddle searches at finite forces, this method also offers insight into force-induced switches of the reaction mechanisms as "catastrophes" where two (or, possibly, more) critical points coalesce. A theory was further developed to analyze force distributions in mechanically stressed molecules and to identify "weak links" or bonds that are likely to break as a result of the applied force. Unlike previous efforts to define forces in molecules, this theory does not rely on highly approximate models (such as molecular mechanics) to describe molecular energies. The theory further predicts a number of yet unobserved phenomena, such as the force multiplication effect where scission of strong bonds can be caused by relatively weak forces.

Mechanical and thermodynamic stability of duplexes formed by strands of a number of unnatural nucleic acid analogs (such as the peptide nucleic acid) was investigated using a combination of umbrella sampling and replica-exchange molecular dynamics. Close correlation was found between thermodynamic and mechanical stability in all cases. While showing good agreement with the existing experimental data, these simulations have further identified several tentative nucleic acid analogs that are capable of forming duplexes with DNA and with themselves, with a stability that far exceed that of wild-type double-stranded DNA.

In conjunction with magnetic tweezers studies of spectrin repeats, molecular dynamics simulations were also performed to study the mechanical stability of those proteins, predicting sequential unfolding mechanism where free energy grows linearly with extension and confirming an earlier theoretical model developed by the PI.

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

In project 1, we have shown that in addition to its well-studied role in controlling developmental gene expression, the nematode nuclear receptor DAF-12 governs expression of a gene network that stimulates aerobic catabolism of fatty acids while simultaneously suppressing anaerobic metabolism. Pharmacologic manipulation of this pathway by targeting DAF-12 or the enzymes that it activates blocks reproductive development. Importantly, this pathway is conserved in parasites, suggesting a novel strategy for treating nematode parasitism. In project 2, we are exploring the tissue-specific actions of FGF21 using organ-selective receptor knockouts. We have shown that the physiologic functions of FGF21, which is secreted from the liver as part of an adaptive response to starvation, are mediated by a neuroendocrine mechanism that involves FGF21 acting on the suprachiasmatic nucleus (SCN) of the hypothalamus. Previously, we also showed that part of the pharmacologic action of FGF21 is through its ability to promote rapid glucose uptake into adipose tissue in obese mice. We now have extended this work to show that another important therapeutic effect of FGF21, the induction of thermogenesis and weight loss, also requires its action in the SCN. The mechanism by which FGF21 governs thermogenesis appears to be by stimulating the release of corticotropin releasing hormone (CRH), which in turn induces sympathetic nerve activity in adipose tissue. The stimulation of CRH is also responsible for FGF21-dependent increases in glucocorticoids. These results identify a hepatic-neuroendocrine circuit that governs nutrient metabolism and it demonstrates that both positive and negative effects of FGF21 are mediated through the CNS.

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

In continuation of our effort to develop mixed ionic-electronic conductors with high catalytic activity for the oxygen reduction reaction (ORR) in solid oxide fuel cells (SOFC) while keeping the thermal expansion coefficient (TEC) matching closely with that of conventional oxide-ion electrolytes, we have systematically investigated various cationic substitutions on the Y and Co sites of the trigonal $\text{YBaCo}_4\text{O}_{7+\delta}$ phase. The major issue with $\text{YBaCo}_4\text{O}_{7+\delta}$ is the severe phase instability at the SOFC operating temperatures of 500–800 °C. We have established that a critical amount of ions such as Zn^{2+} and Fe^{3+} that are stable in tetrahedral sites and a small amount of In^{3+} , respectively, in the Co and Y sites offer excellent long-term phase stability at 500–800 °C, while the substitutions of Ca^{2+} for Y^{3+} or Fe^{3+} for Zn^{2+} enhance the ORR catalytic activity, respectively, due to an increase in the oxidation state of Co and electronic conductivity. For instance, compositions such as $\text{Y}_{0.5}\text{In}_{0.1}\text{Ca}_{0.4}\text{BaCo}_3\text{ZnO}_{7+\delta}$ and $\text{Y}_{0.9}\text{In}_{0.1}\text{BaCo}_3\text{Zn}_{0.6\text{Fe}0.4}\text{O}_{7+\delta}$ display a combination of low TEC, good phase stability, and high catalytic activity. Also, with an aim to suppress/eliminate the deposition of carbon on the surface of Ni catalyst during the operation of an SOFC with hydrocarbon fuels like methane, the incorporation of a small amount (1 atom %) of hydrophilic metal ions like W^{6+} or Sb^{3+} into $\text{NiO-Ce}_{0.8}\text{Gd}_{0.2}\text{O}_{1.9}$ has been explored. For instance, $\text{H}_x\text{WO}_{3-\delta}$ (or $\text{WO}_{3-x-\delta}(\text{OH})_x$) formed on the surface of Ni catalyst by reaction with the water vapor produced during SOFC operation supplies the hydroxyl groups to oxidize carbon and drives it off as carbon dioxide. The mobile protons and oxide ions of $\text{H}_x\text{WO}_{3-\delta}$ facilitates a rapid cleaning of the Ni-catalyst surface. In addition, a microwave-assisted solvothermal process has been developed to access reduced $\text{A}^{2+}\text{V}_2^{3+}\text{O}_4$ (A = Mg, Mn, Fe, Co, and Zn) spinel oxides at low-temperatures of < 300 °C within a short reaction time of 30 minutes. The method is particularly useful to access oxides like $\text{Co}^{2+}\text{V}_2^{3+}\text{O}_4$ that are otherwise inaccessible at higher temperatures under reducing synthesis environments. Finally, the challenge of Sn loss occurring during the sintering process of the light-absorber $\text{Cu}_2\text{ZnSn}(\text{S}_x\text{Se}_{1-x})_4$ has been mitigated by developing a robust film precursor with the addition of ethyl cellulose.

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

With Welch funding, we made substantial progress identifying and measuring the dominant, stable multiprotein complexes shared across the animal kingdom, in the process performing the deepest characterization of animal proteomes on record. With collaborator Andrew Emili (Toronto), we previously developed a strategy (published in *Cell*, 2012) based on deep biochemical fractionation of cells or tissues, analyzing each fraction by tandem mass spectrometry to identify reproducibly co-purifying (hence, likely interacting) proteins. Working with the Emili lab, we have now analyzed >8,000 biochemical fractions from diverse cell, tissue, and whole animal samples from human, mouse, fly, frog, sea urchin, sea anemone, the nematode *C. elegans*, and, as a phylogenetic outgroup, the slime mold *Dictyostelium*. Our initial efforts on the human proteome (*Cell*, 2012) surveyed ~5,500 proteins across ~2,000 fractions; current data exceed ~12,000 proteins (each conserved between humans and other animals) across >8,000 biochemical fractions, encompassing >90 million protein abundance measurements. We automated the analyses of thousands of tandem mass spectrometry datasets using Texas Advanced Computing Center supercomputers, and have now derived a map of hundreds of protein complexes shared across the animal kingdom, defining the biochemical "wiring diagrams" underlying most animal cells. We have found new, uncharacterized protein complexes; initial follow-up experiments show several to be critical to animal embryonic development (e.g., as for one required for proper head and eye development). Over the next year, we are expanding our analysis to measure stoichiometries and subcomplexes.

JOHN T. MARKERT, F-1191, The University of Texas at Austin. SYNTHESIS, MAGNETOCHEMISTRY, AND SUPERCONDUCTIVITY OF METALS AND OXIDES.

Our main activities this year fell into four categories: 1) Magnetic Semiconductors. We have completed in-depth SQUID magnetization studies of ferromagnetism in manganese-implanted germanium films grown on silicon; such materials show promise for incorporating magnetic structures into silicon technologies. This work [*Phys. Rev. Lett.* 112, 126401 (2014)] characterized the dimensionality of spin-glass dynamics, in order to understand long-term magnetic stability in these materials. 2) Nuclear Magnetic Resonance Force Microscopy Experiments. We continued our force-detected NMR measurements in three different probes, studying: a) the temperature dependence the ^{11}B resonance in superconducting MgB_2 crystals, searching for quantum coherence effects; b) ^1H dynamical imaging in microfluids (a precursor to NMR microscopy of biological cells); and c) low-temperature ($T = 0.3\text{ K}$) sub-micron imaging, examining spectral and spatial diffusion of nuclear magnetization. 3) Novel Charge States at Oxide Interfaces. Our pulsed-laser-ablation thin-film growth and studies of epitaxial metal-oxide structures emphasized praseodymium-lanthanum alloy aluminates (001) on strontium titanate (001), which we have found exhibit both Kondo behavior and a nearly two-dimensional metal-insulator transition. 4) Thermal Conductivity of a Quasi-One-Dimensional Spin System. Detailed studies of thermal transport by magnons in a series of samples of $\text{Ca}_2\text{Y}_2\text{Cu}_5\text{O}_{10-\delta}$ with varying oxygen content began to reveal effects of varying spin-chain length on magnetic correlations.

PAUL MARSHALL, B-1174, University of North Texas. KINETIC AND PRODUCT STUDIES OF COMPLEX-FORMING REACTIONS IN THE GAS-PHASE.

Dinitrogen pentoxide is a sink for NO_x in the atmosphere, and homogeneous hydrolysis to yield nitric acid is known to be slow. We have applied computational methods to investigate the thermochemistry and kinetics of this reaction. Geometries and frequencies were obtained via density functional theory, and energies using coupled cluster theory with complete basis set extrapolation. A focus is the pair of torsional modes where rotations of the two NO_2 groups about axes to the central O atom are geared. There is a modest barrier of around 11 kJ mol^{-1} to twisting in opposite directions, while synchronized motion is almost free. This has impact on the entropy and heat capacity of N_2O_5 , which were used to reanalyze literature data on the $\text{N}_2\text{O}_5 = \text{NO}_3 + \text{NO}_2$ equilibrium to obtain $\Delta_f H_{298}(\text{N}_2\text{O}_5) = 14.9\text{ kJ mol}^{-1}$. The preliminary *ab initio* estimate is 13.0 kJ mol^{-1} . The classical barrier to hydrolysis is computed to be 66.5 kJ mol^{-1} which leads to a slower reaction than used in atmospheric models.

Formic acid is an intermediate in the oxidation of methanol and dimethylether in flames, and its reactions with H atoms, O atoms and HO_2 radicals have been investigated computationally. Stationary points were evaluated using the W1 methodology, and rate constants for abstraction pathways at elevated temperatures were obtained using transition state theory. Addition pathways are not important above 400 K.

ANGEL A. MARTI-ARBONA, C-1743, Rice University. RUTHENIUM(II) PHOTOLUMINESCENT PROBES FOR SENSING AMYLOID-B OLIGOMERS IN REAL-TIME.

Recently we discovered that ruthenium dipyrrophenazine complexes present light-switching behavior when exposed to amyloid- β fibrils (*JACS*, 2011, 133, 11121). In the presence of monomeric amyloid- β $[\text{Ru}(\text{bpy})_2(\text{ppz})]^{2+}$ ($\text{bpy} = 2,2'$ -bipyridine, $\text{dppz} = \text{dipyrido}[3,2\text{-a}:20,30\text{-c}]\text{phenazine}$) presents minimum photoluminescence that is enhanced (ca. 50 fold) by aggregated amyloid- β . We have done experiments to elucidate the origin of this photoluminescence enhancement. Binding studies suggest that a single binding site with a dissociation constant of $2.1\text{ }\mu\text{M}$. To elucidate the binding stoichiometry we performed Job plots, which allowed the elucidation a binding site composed of 2.7 amyloid- β monomers per $[\text{Ru}(\text{bpy})_2(\text{dppz})]^{2+}$. In collaboration with Prof Rajeev Prabhakar, we performed molecular dynamic calculations which allowed us to identify a binding site between Phe 20 and Val 18 as the binding site for $[\text{Ru}(\text{bpy})_2(\text{dppz})]^{2+}$. This information has allowed us to propose a mechanism for the light switching behavior of this complex. When $[\text{Ru}(\text{bpy})_2(\text{dppz})]^{2+}$ is in aqueous solution it is non-emissive due to the spontaneous population of a dark-excited state, however when bound to amyloid- β , the microenvironment around $[\text{Ru}(\text{bpy})_2(\text{dppz})]^{2+}$ becomes hydrophobic and the dark state gets destabilized allowing the population of the emissive state.

In addition, we investigated a novel photoluminescence sensor to detect toxic vapors. This sensor is made by immobilizing a ruthenium carbonyl complex within the cavities of zeolite-Y. Treating this material with different solvent vapors produce changes in the emission intensity (vapoluminescence), emission maxima (luminescence vapochromism) and lifetime (vapotemporism). These changes are solvent specific, which allows generating a fingerprint for the easy identification of solvent vapors.

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

A number of important advances were made this past year. We completed the concise syntheses of the aglycone of the anticancer agent IB-00208 and the anticancer alkaloid citrinadin B. We made significant advances toward the synthesis of the anticancer antibiotics of the citreamicin group as well as of the sesquiterpene jiadifenolide, which promotes neurite outgrowth. Intermediates in our total synthesis of actinophyllic acid have been diverted to several compounds that exhibit potent anticancer activity, killing cancer cells faster than established anticancer drugs, while being relatively nontoxic. Quantities of compounds are being prepared for studies in mice. Our general approach to diverse nitrogen heterocycles that may be quickly transformed into novel compounds continues to yield exciting compounds having an array of biological activities. A number of lead compounds having potential for treating cancer, pain, alcohol withdrawal, and Alzheimer's disease have been identified in several collaborations with biologists. In the area of biological molecular recognition, we explored how changes in the structures of small molecules affect energetics, structure, and dynamics in protein-ligand associations. Preliminary studies suggest protein dynamics may play an important role in differential binding energetics for similar compounds. Our primary focus is upon Grb2 and Src SH2 domains and complexes of hepatitis C viral protease with inhibitors.

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

We have made progress in three areas:

1) We have constructed a series of proteasome substrates in which the two components of the proteasomal degradation signal, the ubiquitin tag and the initiation region, are systematically moved away from each other in nano meter steps. We have then measured the rate by which the proteins are degraded. The results suggest that the optimal separation between the two degradation signals is around 3 nm.

2) We have developed methods to construct ubiquitin chains of different geometries by fusing ubiquitin chains enzymatically. We can now make defined ubiquitin chains of two to six ubiquitin moieties and linked through Lys 48 or Lys 63 of ubiquitin. We are collaborating with the laboratory of Dr. J. Brodbelt to characterize these chains by mass spectrometry. We are currently trying to fuse these ubiquitin chains to defined substrates as the ones described under point 1) above. Once we succeed in this step, we will be able to measure degradation of constructs with different degnon spacing and different ubiquitin chains. This will tell us whether the ubiquitin chains affect how the proteasome recognizes the two components of the degradation signal and thus how these components contribute to substrate selection.

3) We have developed methods to follow protein degradation in yeast by making fluorescent protein substrates. These substrates are designed so that the proteasome is forced to initiate at internal disordered regions. We are now trying to adapt these methods to monitor protein degradation *in vitro* with purified proteasome. Eventually, these experiments will reveal how the proteasome recognizes internal sites within substrates.

SEIICHI P.T. MATSUDA, C-1323, Rice University. TERPENE BIOSYNTHESIS.

Classical natural products have been an extraordinarily productive area of chemical research, and the life-changing impact of the molecules isolated from native organisms is widely recognized. However, classical natural products approaches are limited to providing the compounds that the organisms accumulate. Many plant defense compounds are produced only in response to herbivores or infection, and they are consequently inaccessible to classical extractive approaches. We have previously used genome mining approaches to identify all of the 13 oxidosqualene cyclases in the model plant *Arabidopsis thaliana* and determine the structures of their 50 products. More detailed analyses establish that the enzymes PEN1, PEN3, and PEN6 generate the most diverse oxidosqualene cyclase product profiles known, and we are preparing manuscripts describing this work. We are also expanding this approach to establish the ability of a variety of other plants to synthesize terpenoids. The number of sequenced plants is now approaching 50, and initial assessment of the genes these organisms encode establishes that *Arabidopsis'* ability to make triterpenoids is actually more modest than is typical in the dicotylenous plants.

KATHLEEN S. MATTHEWS, C-0576, Rice University. GENETIC REGULATORY PROTEINS: STRUCTURE-FUNCTION relationships.

Genetic regulatory proteins are key players in modulating transcription of DNA for all organisms. We are engaged in studies of a prokaryotic genetic regulator, lactose repressor (LacI) found in *E. coli*, and a eukaryotic transcriptional regulatory protein, Ultrabithorax (Ubx) found in *Drosophila*. LacI recognition and affinity for its target site in the DNA is responsive to the presence of sugars, for which binding elicits a structural transition that impedes recognition of the target DNA sequence. A temperature-sensitive LacI variant was incorporated into a synthetic gene oscillator, and the temperature-independence of this system indicates compensation for the normal Arrhenius effects on reaction rates. Thus, genetic circuits can exhibit robust response to external environmental conditions, as observed for the resistance of circadian rhythms to temperature fluctuations. In contrast to LacI, Ultrabithorax contains both a well-folded DNA-binding domain and intrinsically disordered regions that can selectively bind a variety of protein folds. Using specific and often overlapping sequences, Ubx binds to a wide range of partner proteins. In addition to the potential for competition between partners, modulation of partner binding results from alternative splicing of Ubx mRNA to vary inclusion of specific sequences. Beyond partner binding, disordered regions may also be responsible for *in vitro* assembly of Ubx fibers that retain DNA binding capacity. Results with multiple protein fusions demonstrate that adding other proteins to the N-terminus of Ubx does not impede its assembly into fibers, providing interesting avenues for creating functionalized materials in a single step.

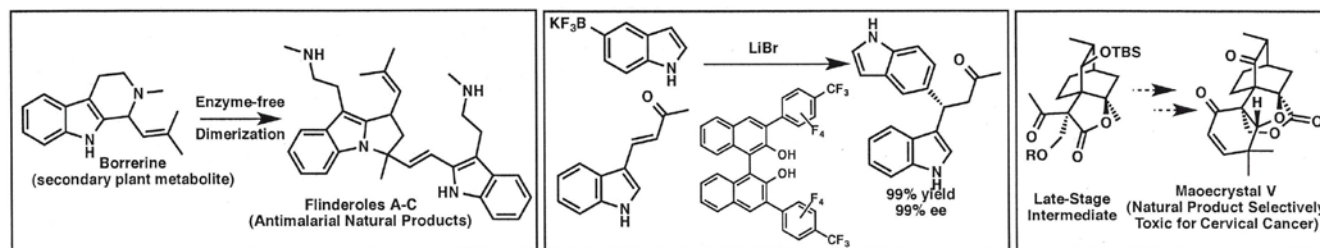
JEREMY A. MAY, E-1744, University of Houston. THE TOTAL SYNTHESIS OF BIOACTIVE NATURAL PRODUCTS VIA NOVEL STRATEGIES.

Clarification of the biosynthesis of the antimalarial Flindersia alkaloids was made. Whereas previous specific rotation data seemed to suggest that the flinderole natural products (see first figure) were isolated as single enantiomers, we showed that the original data was unreliable, and we obtained the true values for the specific rotation of enantiopure samples (*Tetrahedron Lett.* 2013). This supports our proposed enzyme-free biosynthesis. We have also made progress in the synthesis of antimalarial analogs of these compounds.

We expanded the substrate scope and performed mechanistic work for our carbene/alkyne cascade that terminates in C-H bond insertion (*Tetrahedron* 2014). Thus, highly caged structures found in natural product cores are now accessible, and diazoketones were shown to be excellent substrates. We have successfully also incorporated this reaction as the key step for the synthesis of Brazilide A.

The enantioselective conjugate addition to heterocycle-appended enones has been made compatible with trifluoroborate salts, whose greater reactivity allow the use of aryl boronates as nucleophiles (see second figure). Fluoride dissociation was discovered to be a key mechanistic step, and the reaction was used as a key step in the synthesis of Discoipyrrole D (communication submitted).

Lastly, we advanced the synthesis of maoecrystal V to a key late-stage intermediate (see last figure). Key physical organic effects that control C-H bond insertion have been elucidated. Construction of the final cyclohexene ring has progressed, and we are preparing a communication to report the success of this strategy.



JENNIFER A. MAYNARD, F-1767, The University of Texas at Austin. CONTROL OF PROTEIN FOLDING QUALITY CONTROL IN THE BACTERIAL PERIPLASM.

During year three of funding, we have been working on more complex aspects of Aims 2 and 3 of the project: Predict Skp-sensitive proteins in the genome based on biophysical parameters and Create substrate-specialized Skp variants via directed evolution techniques. We have reported the results in three recent papers and one submitted manuscript. During 2013-14, this grant supported two graduate students and one superb undergraduate student, who began graduate school at Stanford University. Skp is an important protein-folding chaperone involved in biogenesis of bacterial outer membrane proteins that is being increasingly recognized for its role in assisting soluble protein folding in the crowded environment of the bacterial periplasm. Using bioinformatics tools and the sequences of known Skp-sensitive and Skp-insensitive proteins, we have made genome-wide predictions about proteins that are likely to interact with Skp and are currently testing these predictions. It appears that Skp is a structurally unique, yet functionally homologous chaperone to the well-known cytoplasmic GroEL chaperone. We used this knowledge to assist in recombinant production of a large bacterial toxin, the adenylate cyclase toxin and create a number of variants to explore the unique folding properties of this protein. We have also created a panel of proteins with systematic changes in electrostatic charge to probe the effects of protein surface charge on behavior in highly concentrated, cell-like conditions. Under these conditions, protein form discrete nanoclusters of defined size. Our current hypothesis is that shape and charge will dictate cluster size in a given buffer pH.

OGNJE Š. MILJANIĆ, E-1768, University of Houston. CONJUGATED BENZOBISOXAZOLE CRUCIFORMS AS FLUORESCENT SENSORS IN SOLUTION AND SOLID STATE.

1. We have performed exhaustive characterization of photophysical properties of benzobisoxazole cruciforms, which established that members of this class of fluorophores can cover almost the entire visible range in terms of emission, occasionally with fluorescence quantum yields as high as 80%.
2. We have developed a protocol which prepares multiple pure value-added esters starting from a complex mixture containing as many as 16 starting materials, through an iterative reactive distillation protocol. This self-sorting methodology holds promise for applications in basic chemical and fragrance industries
3. We have created perfluorinated metal-organic frameworks (MOFs), characterized by unique adsorption properties and superhydrophobicity. We are presently working on incorporating other sophisticated functional organic precursors into MOFs.
4. In the domain of chemical education (which is the theme of this year's Welch Conference), we have (a) published a protocol for facile conversion of crystal structure data into physical 3D printed models (highlights in *C&E News*, *CrystEngComm* cover page, and *Chemistry World*), and (b) disclosed a video procedure for the use of our fluorophores in qualitative analyses of carboxylic acids, boronic acids, and amines—some of which are of pharmaceutical interest.

NANCY S. MILLS, W-0794, Trinity University. NOVEL APPROACHES TO THE SYNTHESIS OF ANTIAROMATIC DICATIONS AND DIANIONS.

Antiaromatic dianions: The NMR studies of the deprotonation of benzylidene [2.3]benzocycloheptatriene demonstrate conclusive proof of the formation of both the mono- and antiaromatic dianion. Substantial progress on the synthesis of precursors to homo dimers of the antiaromatic benzannulated cycloheptatrienyl anion, in which the benzannulation is varied on the 7-membered ring. We have in hand the precursor to the homo-dimer with benzannulation in the [2.3] position.

Antiaromatic dications The antiaromaticity of bis-indenylidene dications can be modified by changing the manner in which the indenyl systems are linked. We have made progress in the examination of substituted 1,1'-linked and 5,5'-linked bisindenylidene dications. In the first system, we have overcome difficulties in coupling indanones to give the parent bis-indene. In the second system, we have made substantial progress on the preparation of the precursor to a dication with phenyl substitution in the 6-membered ring of the indene. The behavior of this dication will complement the behavior of dications already prepared with substitution in the 5-membered ring of the indenyl system.

Examination of delocalization: Charged antiaromatic species show a tension between the desire for increased delocalization of charge and the need for antiaromatic species to reduce their antiaromaticity through a decrease in delocalization. Calculations show that charge is a better measure of delocalization than is bond length alternation.

Note: My publication record this past year is thin. This is a conscious decision. I will retire at the end of the next academic year. These last years are the last opportunity for my experimental work, so I have emphasized lab work over writing, which can, and will, be done in retirement. As evidence of that, this summer I have a research group of fifteen undergraduates, four supported by the Foundation, a post-doc and a technician, the largest research group of my career and arguably one of the largest research groups at an undergraduate institution in the country.

EMILIA MOROSAN, C-1791, Rice University. NOVEL PHASES AND GROUND STATE IN VALENCE-FLUCTUATING INTERMETALLICS.

(1) We were successful in growing for the first time single crystals of YbRh_3Si_7 (1-3-7). Preliminary measurements on YbRh_3S_7 reveal that this is indeed a new HF. In addition to fully characterization of the chemical and physical properties of this compound, we will direct part of our search towards potential 1-3-7 superconductors (SCs). This will then allow us to directly probe what happens in the solid solution of HF and SC analogues.

(2) For the first time, we successfully synthesized single crystals of several 3-4-13 compounds $\text{R}_3\text{T}_4\text{Ge}_{13}$, with $\text{R} = \text{Y}, \text{Yb}$ or Lu , $\text{T} = \text{Co}, \text{Rh}, \text{Ir}$ or Os . Of these, four are new SCs, $\text{Lu}_3\text{T}_4\text{Ge}_{13}$ ($\text{T} = \text{Co}, \text{Rh}, \text{Os}$) and $\text{Y}_3\text{Os}_4\text{Ge}_{13}$. The superconducting state emerges from a poor metal state, which is likely due to the complex crystal structure modification which occurs in the 3-4-13 germanides, as shown by detailed crystallographic measurements and analysis (manuscript submitted to *Chemistry of Materials*).

The Yb 3-4-13 compounds ($\text{I} = \text{Co}, \text{Rh}, \text{Ir}$) show intermediate valence ("IVal") behavior for the Co and Rh analogues, while the Ir one is a new HF, consistent with most Yb being trivalent in $\text{Yb}_3\text{Ir}_4\text{Ge}_{13}$, but also in the Ir-rich Rh doped analogues. Most surprising is the tendency towards Yb^{3+} and HF behavior upon doping the "IVal" compound $\text{Yb}_3\text{Rh}_4\text{Ge}_{13}$ with non-magnetic Lu. The manuscript on these 3-4-13 "IVal" and HF compounds will be submitted to *PRB* in the next month.

(3) Single crystals of $\text{Yb}(\text{Sb}_{1-x}\text{Bi}_x)_2$ have recently been grown, to be measured in the next months.

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

Over the past year we have conducted experimental investigations of (1) the lithiation/de-lithiation and sodiation/de-sodiation of nanoparticles and solid nanostructured thin films, (2) the photoelectrochemistry of water oxidation and reduction by visible light using nanostructured metal-oxide semiconductors as the light absorber with electrocatalysts, (3) the surface chemistry of catalysis, particularly as it pertains to gold. The idea of room temperature sodium ion batteries has recently taken off and we have performed several studies related to this science. Cathode hosts seem to be somewhat readily available but anode hosts are scarcer, so our work focused on anode materials and chemical architectures. Additionally, we reported several other studies regarding lithiation/delithiation in hosts with high capacities and capable of high rates with good cyclability. Several studies of molecular transformations on gold and gold-palladium surfaces were conducted since these catalysts show great promise at low temperatures. Finally, much work was published regarding photo-assisted water oxidation and reduction. These latter efforts involved the search for both stable semiconducting light-absorbers as well as electrocatalysts.

SIEGFRIED MUSSER, BE-1541, Texas A&M University System Health Science Center. STRUCTURE OF THE NUCLEAR PORE PERMEABILITY BARRIER BY SUPER-RESOLUTION MICROSCOPY.

The ~50 nm diameter pore of nuclear pore complexes (NPCs) is filled with a network of intrinsically unfolded polypeptides, which create a permeability barrier. In total, these polypeptides contain thousands of phenylalanine-glycine (FG) repeats, which are the binding motifs for soluble nuclear transport receptors (NTRs) that carry cargos through the NPC. Due to its amorphous and highly flexible nature, deciphering the structural and functional properties of the FG-network has been a formidable challenge. Over the past few years, we developed a novel technique, termed polarization photoactivated localization microscopy (p-PALM), to measure the rotational mobility of individual molecules. The photoactivatable fluorescent probe, mEos3, covalently tethered within the FG-network is used to report on the local environment. This past year, we performed mathematical calculations and rotational random walk simulations to develop models describing the effects of the covalent tether and the 'effective viscosity' of the local FG-network on the rotational mobility of the mEos3 probe. The simulations indicated important parameters for data collection, prompting improved data acquisition protocols. p-PALM measurements indicate that the importin β NTR and the transport inhibitor wheat germ agglutinin inhibit rotational mobility – the effects of the latter are much stronger. While these results verify binding, additional work is required to determine proximity and affinities. Ultimately, p-PALM measurements on the mEos3 probe individually attached to all 11 FG-polypeptides in multiple locations will allow us to estimate the location and local density of the EG-polypeptides throughout the FG-network, which are essential for building an accurate model of the permeability barrier.

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

We made significant progress this year toward our objectives. First, collaborating with quantum chemistry theorists, we established that the parabolic shifts downward in energy of some C60 vibrational modes are the result of bias-driven molecule-electrode partial charge transfer. The modes soften as the occupancy of an antibonding molecular orbital is increased under voltage bias. This work was published in *PNAS*. We also used the temperature dependence of the electrical resistivity of our electrodes as a clever *in situ* thermometer to assess how much local heating due to laser illumination was taking

place in these experiments. Under conditions of interest, the temperature rise was limited to a few Kelvin. Through the dependence of the plasmon response on incident polarization, we could determine the fractions of temperature rise due to plasmons and direct absorption. This work was published in *Nano Lett.*

Our investigations into using our nanogap structures for surface-enhanced infrared absorption at the few-molecule level showed that achieving this goal will require new instrumentation (dedicated FTIR system). We have continued to investigate gate-dependence of SERS response, though it has been challenging to produce devices that simultaneously exhibit both gate modulation of the molecular redox state and SERS response. We have worked with PCBM (a C60 derivative possessing a built-in dipole), and have demonstrated that we can see both the bias-driven charge transfer shifts observed in C60, and linear-in-voltage true vibrational Stark effect in single molecules. We are preparing this work for publication.

JOSEPH B. NATOWITZ, A-0330, Texas A&M University. NUCLEAR REACTION STUDIES.

Using 7.5 MeV/nucleon ^{197}Au projectiles incident on a ^{232}Th target, we have continued investigating alternative reaction pathways for heavy element production. Our experiments are based upon the detection of alpha particle decays from recoiling heavy element reaction products implanted in an inert catcher foil. - The ^{197}Au beam was pulsed at different intervals in order to be able to identify species of different half-life. High alpha-energy, very heavy element candidate decays were observed. Using 3D printer technology we have now constructed a new eight Ionization Chamber detector array and, with our colleagues at the Jagiellonian University, Krakow and Silesian University, Katowice, a sophisticated active catcher system consisting of a high granularity array of scintillators read by photomultiplier tubes (See Fig. 1) . This allows correlation of a detected alpha decay with implantation position and the observation of multiple decays from the same recoil implantation site (decay chains from a heavy parent nucleus). New experiments using ^{197}Au and ^{238}U beams from the TAMU K500 Cyclotron are scheduled to begin on 28 August 2014. Tests of SCVD diamond detectors as potential replacements for the scintillators are also underway. Such detectors will provide much better energy resolution and isotope identification.

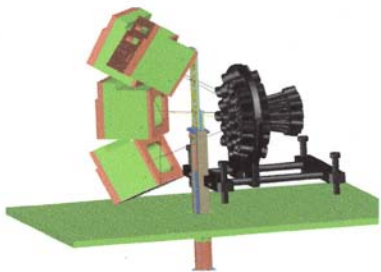


Figure 1: New experimental array. Not all IC detectors are shown. Beam enters from left.

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

Ruthenocuprates, $\text{RuSr}_2\text{R}_{2-x}\text{Ce}_x\text{Cu}_2\text{O}_{10-d}$ with $\text{R}=\text{Gd}, \text{Eu}$ exhibit coexistence of superconductivity and weak ferromagnetism. They also exhibit granular superconductivity due to their granular structure (a 3-D ensemble of small superconducting grains, weakly coupled by an inhomogenous intergrain medium which can be modeled as a 2-component system). We have previously demonstrated that this granular behavior leads to crossing point behavior in both thermodynamic and dynamic properties, i.e. that the property $P(x,y)$ where x and y are the thermodynamic variables, intersect strictly at a single point when values of P are plotted as a function of one variable for different values of the other. This year we have developed a new granular system $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ (YBCO) nucleated on randomly distributed CeO_2 nanoparticles. By controlling the size of the nanoparticles and their concentration relative to YBCO, we can vary the effective dimensionality of the granular superconductor. Studies of the effect of dimensionality on crossing point behavior are in progress. We have also studied STM tip-sample interactions with graphite to prepare controllable misoriented graphene superlattices in collaboration with Jiakai Nie at Beijing Normal University, China.

ANDRIY NEVIDOMSKYY, C-1818, Rice University. MAGNETIC ANISOTROPY AND ORDERING IN MOLECULAR AND SOLID-STATE MAGNETS: FIRST-PRINCIPLES CALCULATIONS AND EFFECTIVE SPIN THEORY.

Both aforementioned objectives have been successfully achieved. **Objective 1:** A relativistic DFT approach was used for spin-orbit coupling. Together with a graduate student, Vaideesh Loganathan, we have implemented two different methods of calculating magneto-crystalline anisotropy energy (MAE) from first principles. The first method involves calculating brute force the difference in total energy between two spin configurations. While most accurate, it is computationally expensive. The second approach, the so-called "torque method," relies on performing only one calculation: the derivative of the total energy with respect to angle $dE/d\theta$, for the direction of the magnetization at $\theta=45^\circ$ angle to the easy axis. Both methods were tested on Fe_2P , for which MAE has been previously calculated, and then applied it a novel material $\text{Fe}_{1/4}\text{TaS}_2$ synthesized in E.Morosan's lab at Rice. **Objective 2:** With a student Patricia Ergueta, we have explored various spin-wave theories of a magnet, focusing on quantum corrections. We have benchmarked and successfully applied these methods to explain spin-wave dispersion in the Fe pnictide class of materials, where a wealth of neutron scattering data is available. We found that the recently (2013) developed generalized spin-wave theory is very effective at capturing the spin physics. The results will be soon submitted for publication. The PI has also published or submitted several articles relevant to spin physics in Fe pnictides.

KYRIACOS C. NICOLAOU, C-1819, Rice University. SYNTHESIS OF BIOLOGICALLY ACTIVE MOLECULES.

During the past grant period, progress has been made toward the synthesis of biologically active molecules as follows:

- a. Synthesis of Δ^2 -prostaglandin J_3 (Δ^2 -PG J_3), a recently isolated substance with potent anti-leukemia properties. Our synthesis rendered this scarce natural molecule readily available for further biological investigations and possible development as an anticancer drug. Several analogs have also been designed and synthesized and are currently being evaluated for their anticancer activities.
- b. Synthesis of a number of maitotoxin fragments have been synthesized and are currently being coupled to produce larger domains of the molecule.
- c. Progress towards the trioxacarcins has been made with several building blocks and advanced intermediates constructed and poised for further elaboration.
- d. A number of novel analogs of the naturally occurring antibiotic, viridicatumtoxin B have been synthesized and tested for antibacterial properties. Some of them exhibited equal or higher potencies against drug resistant bacterial stains (e.g. methicillin resistant *Staphylococcus aureus*, MRSA; vancomycin resistant *Enterococcus faecalis*), despite their simpler structures.

QIAN NIU, F-1255, The University of Texas at Austin. GAP OPENING BY SYMMETRY BREAKING IN GRAPHENE SYSTEMS.

We investigated gap opening in graphene by proximity coupling to an antiferromagnetic insulator, and found a quantum anomalous Hall phase. Inspired by our earlier work on graphene systems, we also investigated magnetic control of the valley degrees of freedom in transition metal dichalcogenides, and studied topological classification of 2D crystalline insulators with space group symmetry. In addition, we conducted research on spintronics issues in ferromagnetic as well as antiferromagnetic materials including those with non-collinear spin arrangements. Finally, we report a theoretical breakthrough in extending our semiclassical theory to second order in the fields.

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

We have continued our investigations of plasmon-enhanced light harvesting processes with metallic nanoparticles. The major accomplishments include an explicit demonstration of plasmon-induced photodissociation of H₂ on gold nanoparticles deposited on an inert glass surface, the development of a plasmonic nanoantenna providing sufficient light concentration to enable coherent anti-Stokes Raman scattering with single molecule sensitivity, the demonstration of gain for plasmon propagation in strongly confined silver nanowires, and the development of tunable plasmonic nanoparticles with high-index facets for photocatalysis. Other major achievements include the development of a method for synthesis of three-dimensional metallic nanoparticle clusters, a method for fabrication of porous tunable metallic nanoparticles, scalable colloidal lithography for fabrication of split ring resonator substrates, investigations of how the cross section of metallic nanowires and nanobelts influence the plasmon propagation length, and a demonstration that an array of graphene nanodisks can serve as a highly tunable absorber. We have demonstrated strong quantum mechanical and nonlocal effects in concentric core-shell structures and nanowire dimers with narrow gaps. We have made significant progress in developing aluminum as a low-cost and abundant plasmonic material by demonstrating the tunability of the plasmon resonances of Al nanoparticles across the UV and visible part of the spectrum. Finally in the context of biological and medical applications we have demonstrated large fluorescence enhancements in bimetallic particles.

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

We have identified the role that excited state dynamics can play in roaming systems, recently identified for the first time by our group in the nitrate radical photochemistry. We have since made significant progress towards demonstrating that roaming may mediate excited state processes by extending our studies to other systems. We postulate that multistate roaming should be prevalent in open-shell systems and are pursuing the study of the challenging CH₂NO₂ radical photochemistry. One important result of our work is that product vector correlations can be observed in roaming systems, and therefore, provides a window into the stereodynamics of important bimolecular reactions. We have built on our method to extract speed-dependent vector correlations from sliced ion images, extending the method to include multiphoton detection. This should enable a broader application of the technique, specifically to a wider range of chemical systems which will ultimately provide a stringent test for modern theoretical chemistry and increase of understanding of chemical reactivity.

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

Our previous aims for understanding how heme proteins regulate absolute ligand affinity, discrimination between O₂, CO, and NO, and rates of ligand uptake and release have been achieved. Over the past four years, the exact pathways for ligand entry and exit into three monomeric heme proteins and one tetramer (sperm whale Mb, the mini-hemoglobin from the Nemertean worm *Cerebratulus lacteus*, the truncated hemoglobin from *Bacillus anthracis*, and tetrameric human HbA) were determined by mutagenesis mapping and time resolved X-ray crystallography. Our remaining goals are to evaluate the related stereochemical mechanisms for autooxidation, dissociation of heme, and unfolding of these heme proteins and the reverse processes involved in holo-heme protein assembly. Using past results, we have derived a mechanism for autooxidation of human HbO₂, which includes both unimolecular dissociation of HO₂• and bimolecular reaction of O₂ with a transient hexacoordinate heme species and explains the dependence of the rate of autooxidation (k_{autox}) on [O₂] and pH. We have developed new experimental methods to measure more directly differences between the α and β subunits in tetrameric HbA and to evaluate the structural causes of the dramatic 10 to 30-fold decreases in k_{autox} when HbA dimers either associate to form native tetramers or bind to the serum protein,

haptoglobin. We have also developed a cell-free globin gene transcription and translation system that is allowing us to: (1) obtain quantitative correlations between apoglobin folding parameters and holo-globin expression yields, and (2) evaluate computational models that attempt to predict mutations that will increase apoglobin stability and assembly with heme.

MOHAMMAD A. OMARY, B-1542, University of North Texas. MOLECULAR SPECTROSCOPY AND BONDING OF COORDINATION COMPOUNDS: MORE OUTSTANDING ISSUES AND NEW ADVANCES.

An experimental and computational study of correlations between solid-state structure and optical/electronic properties of cyclotrimeric gold(I) carbeniates, $(\text{Au}_3(\text{RN}=\text{COR})_3)$ ($\text{R}, \text{R}' = \text{H}, \text{Me}, {}^n\text{Bu}$ or ${}^i\text{Pr}$) is reported. Synthesis, structural and photophysical characterization of novel complexes $[\text{Au}_3(\text{MeN}=\text{CO}^n\text{Bu})_3]$, $[\text{Au}_3({}^n\text{BuN}=\text{COMe})_3]$, $[\text{Au}_3({}^n\text{BuN}=\text{CO}^n\text{Bu})_3]$ and $[\text{Au}_3({}^i\text{PrN}=\text{COMe})_3]$ is presented. Changes in R and R' lead to distinctive variations in solid-state stacking, luminescence spectra and conductive properties. Solid-state emission and excitation spectra for each complex display a remarkable dependence on the solid-state packing of the cyclotrimers. The electronic structure of $[\text{Au}_3(\text{RN}=\text{COR})_3]$ was investigated via molecular and solid-state simulations. Calculations on $[\text{Au}_3(\text{HN}=\text{COH})_3]$ models indicate that the infinitely extended chain of eclipsed structures with equidistant Au--Au aurophilic bonding can have lower band gaps, smaller Stokes' shifts and reduced reorganization energies (λ). The action of one cyclotrimer as a molecular nanowire is demonstrated via fabrication of an organic field effect transistor and shown to produce a p-type field effect. Hole transport for the same cyclotrimer-doped within a poly(9-vinylcarbazole) host - produced a colossal increase in current density from ~ 1 to ~ 1000 mA/cm². Computations and experiments thus delineate the complex relationships between solid state morphologies, electronic structures and optoelectronic properties of gold(I) carbeniates.

We also proved the cooperativity of metallophilic and excimeric bonding and their consequences on absorption and phosphorescence energies and photo-induced magnetism for group 12 clusters.

JOSÉ ONUCHIC, C-1792, Rice University. EXPANDING THE PROTEIN FOLDING LANDSCAPE TOWARD BIOMOLECULAR MACHINES.

Our structure-based models (SBM) have been successful not only in protein folding but also in modeling molecular motors. Structural information, however, is limited, particularly about all different functional configurations. This is a major limitation for SBM's. Our statistical methods to study amino acid coevolution (Direct Coupling Analysis - DCA) provide additional information useful to study structure and function. During this second year, we combined these two methods (SBM and DCA) to create a novel way to investigate the mechanisms associated to folding and function: 1) Utilizing this combined approach we were able to determine several intermediates or hidden states that are of functional importance for different enzymes, signaling proteins and motors, which would be impossible simply by SBM's. 2) We explored the mechanistic aspects of protein translocation in the integral membrane protease FtsH. Dual basin-SBM simulations (open and closed state) reveal a functionally important paddling motion in the catalytic cycle. DCA predicts physical contacts between AAA and peptidase domains of the motor, which are crucial for the open to close transition. Our integrated methodology can explore the functional landscapes of complex biological macromolecules previously inaccessible to methods dependent on experimental structural information.

KIM ORTH, I-1561, The University of Texas Southwestern Medical Center. ELUCIDATE THE BIOCHEMICAL MECHANISM USED BY *Vibrio* VopQ TO INDUCE AUTOPHAGY.

Over the last year we have continued our studies on the biochemical activity of VopQ. We previously demonstrated *Vibrio parahaemolyticus* uses the Type III effector, VopQ, to alter autophagic flux by manipulating the partitioning of small molecules and ions in the lysosome. We next show that the accumulation of autophagic vesicles is due the fact that VopQ is a potent inhibitor of vesicular membrane fusion based on an *in vitro* membrane fusion model. VopQ inhibits the final step of membrane fusion by inhibiting trans-SNARE complex formation. Furthermore, we identified a unique mutation that delineates the two inhibitory functions of VopQ, deacidification and membrane fusion, thereby, supporting our hypothesis that the inhibition of membrane fusion is independent of VopQ's pore-forming activity. Future studies involve structural analysis of VopQ.

OLEG V. OZEROV, A-1717, Texas A&M University. HIGHLY UNSATURATED CATIONIC GROUP 10 TRANSITION METAL Pincer COMPLEXES.

Our approach to generation of highly reactive transition metal cations relies on using cationic main group reagents to abstract halides or pseudohalides from the coordination sphere of a neutral transition metal precursor. Silylium cations partnered with halogenated carborane anions are particularly well suited to this purpose. We conceived of covalently linking the silylium cation with the carborane anion and were able to synthesize such a zwitterionic molecule that gives the advantage of being a well-defined molecular reagent that acts as a silylium cation.

On the other hand, the nature of the pincer ligand supporting the transition metal is critical in enabling a truly unsaturated cation. We have synthesized a broad array of diarylamido-based PNP- and PNN-type pincer ligands and explored their electronic properties. This work allows us to better design ligands for new cationic complexes that may allow for triplet ground states of such cations and give rise variable Lewis acidity.

Our understanding of the ligand space led us to synthesize new pincer ligands based on the carbazole backbone (in place of diarylamido) for our efforts in accessing a cationic methane complex of Pt. Carbazole is less easily oxidized and less basic than a typical diarylamine and should provide a more robust supporting framework.

In addition, partial support from the Welch Foundation grant has helped advance a few related projects over the last year. This especially pertains to the chemistry of pincer-supported unsaturated Rh fragments that are isoelectronic to our target cationic complexes of group 10 metals.

KEITH H. PANNELL, AH-0546, The University of Texas at El Paso. CATENATED GROUP 14 COMPLEXES.

Our studies on the transition metal-catalyzed silane (R_3SiH) reduction of amides to amines has uncovered the versatility of the siloxymethyl-dimethylamine intermediates. $R_3SiOCH_2NMe_2$ (**1**), as hidden Eschenmoser's reagents. Thus, the reactivity of **1** with molecules containing active RE-H bonds, E = O, S, and R_2NH result in the ready aminomethylation of the E moiety, i.e., $RSCH_2NMe_2$, $ROCH_2NMe_2$, and $R_2NCH_2NMe_2$, respectively. The silicon-containing product is R_3SiOH and the h-containing products are readily obtained *via* distillation. We also observed the capacity of silanes to effectively transform $C1CH_2NMe_2$ to Me_3N , a further example of the utility of silanes as reducing agents.

Attempts to form unsymmetrical disiloxanes, $Me_3SiOSiR'_3$ from the trapping of **1** directly via the molybdenum-catalyzed reaction of R_3SiH and DMF in the presence of Me_3SiCl , led to the predominant formation of $Me_3SiOSiMe_3$. We propose that a highly unusual trimethylchlorosilane activation by DMF leads to $[Me_3SiO]^+ [Me_2N=CHCl]^-$, followed by the nucleophilic attack of $[Me_3SiO]^-$ on Me_3SiCl resulting in predominant formation of the observed $Me_3SiOSiMe_3$.

CHANDRASHEKHAR PASARE, I-1820, The University of Texas Southwestern Medical Center. BIOCHEMICAL ROLE OF IRAK-1 REGULATED CASPASE-1 ACTIVATION AND CLEAVAGE.

In the past year, we made significant progress in understanding the role of TLR signaling in regulating rapid NLRP3 inflammasome activation. We discovered that when macrophages encounter a TLR and NLRP3 ligand simultaneously, this leads to rapid cleavage of caspase-1. More importantly we discovered that IRAK-1, a signaling molecule downstream of TLRs is responsible for regulating NLRP3 inflammasome activation and caspase-1 cleavage. Furthermore we found that IRAK-1 physically associates with both NLRP3 and its adapter molecule ASC. Absence of IRAK-1 completely abrogated the ability of macrophages to induce rapid caspase-1 cleavage. In the next set of experiments we discovered that this pathway is not only important for detecting soluble ligands of TLRs and NLRP3, but that IRAK-1 dependent caspase-1 activation is important for the ability of macrophages to respond rapidly to *Listeria monocytogenes* infection, both *in vitro* and *in vivo*. IRAK-1 is a serine threonine kinase and the importance of its kinase activity has never been discovered. We next hypothesized that the kinase function of IRAK-1 could be important for rapid NLRP3 inflammasome activation. Use both biochemical (IRAK-1 kinase inhibitor) and genetic (a mouse expressing kinase dead knock in of IRAK-1) approaches, we were able to demonstrate that the kinase activity of IRAK-1 is indeed important for regulating caspase-1 cleavage following NLRP3 inflammasome activation. There are two outstanding questions that are the subject of current investigation in the lab. We have successfully made various truncations of IRAK-1 to characterize the domains of IRAK-1 that interact with NLRP3 and ASC and we have also initiated experiments to identify the substrates phosphorylated by IRAK-1. We expect to have several candidates soon that can then be investigated for their importance in regulating NLRP3 inflammasome activation. The findings described above have been successfully published in the *Proceedings of National Academy of Sciences* earlier this year.

MATTEO PASQUALI, C-1668, Rice University. PHYSICAL CHEMISTRY OF GRAPHENE FLUIDS.

In the past year, we have continued research into the fundamental physical chemistry of dispersed nanoparticle fluids as well as exploring the relationship between solution behavior and nanoparticle self-assembly into solid-state materials such as fibers, films, and foams. In addition to previously reported dispersions of carbon nanotubes (CNTs) and graphene in superacids, we have also investigated different solvent systems for nanoparticle fluid studies. We reported a novel dispersion method for CNTs as crown ether-stabilized polyelectrolytes in organic solvents; the behavior of which is an interesting corollary to CNT superacid solutions. Additionally, the behavior of large and small graphene oxide flakes was studied in aqueous solutions.

Because of the influence nanoparticle geometry has on the resulting physical chemistry of their solutions, precise characterization of their size is vital. To this end, we investigated techniques for nanoparticle size measurements through direct imaging of solutions using cryo-electron microscopy and bulk solution viscosity measurements.

Finally, our desire to study mixed nanoparticle solution behavior has led to ongoing development of dispersion methods for non-CNT nanoparticles, notably graphene, graphene nanoribbons, and boron nitride nanotubes. Initial results have shown that mixed graphene-CNT and graphene nanoribbon-CNT solutions can be self-assembled into blended 3D materials, and additional investigations into these solutions are underway.

JEAN-PHILIPPE PELLOIS, A-1769, Texas A&M University. DETERMINATION OF THE MECHANISMS BY WHICH LYTIC PEPTIDES DISRUPT LIPID BILAYERS.

In this grant year, we have established that arginine residues are key mediators of the interactions between lytic peptides and negatively-charged phospholipids. We have also established that oxidized phospholipid is far more susceptible to the activity of cell penetrating peptides than their non-oxidized counterparts. Indeed, arginine-rich peptides aggregate with oxidized unsaturated lipids and that aggregation is accompanied by leakage at low peptide to lipid ratio. These results are important because oxidized lipids are components of cellular membranes under oxidative stress. Our results therefore suggest that oxidation of membranes is an important contributor of lipid bilayer penetration and permeation.

In addition, our work on lytic peptides has led to the discovery of a new compound named "dfTAT" which can cause the leakage of specific cellular membrane. This compound is in turn useful as a tool for the delivery of proteins inside cells. This new methodology is published in the high impact journal *Nature Methods*.

MARGARET A. PHILLIPS, I-1257, The University of Texas Southwestern Medical Center. ENZYME CATALYZED HYPUSINE MODIFICATION IN THE PROTOZOAN'S PATHOGEN *Trypanosoma brucei*.

In past fund years we showed that DHS is an essential protein in *T. brucei* and identified a unique regulatory mechanism for controlling DHS activity. To understand the function and role of hypusine modification in *T. brucei* we generated eIF5A RNAi knockdown lines and showed that eIF5A is essential for growth of both the blood and insect stage parasites. Cell growth was rescued by expression of a complementing plasmid containing human eIF5A but not by a Lys50Ala mutant that is unable to be modified by hypusine, showing that hypusine modification of eIF5A is essential for its function. It was recently shown that eIF5A and the bacterial equivalent EF-P promote translation of poly-proline motifs by relieving ribosome stalling that occurs at these sequences. We used bioinformatics to identify proteins containing polyproline stretches of three or more in *T. brucei* identifying 1210 of 7835 predicted proteins. Interestingly, well represented in the list are cysteine peptidases that contain stretches of eight prolines, zinc finger proteins with stretches of six, and many actin-related proteins. One of the standout actin-related proteins is a putative formin that contains a stretch of 10 prolines. We showed that the expression of formin was reduced after knockdown of eIF5A, supporting the role of eIF5A in translation of polyprolyl containing proteins. The concentration of polyprolyl repeats in actin related proteins, which are essential for parasite growth, undoubtedly contributes to the efficacy of polyamine biosynthetic inhibitors, which are used for treatment of African sleeping sickness.

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 for 2010-2013: 1) symmetrized Gaussian (SG) basis set methods; 2) quantum trajectory methods (QTM); 3) molecular applications. The last year has seen truly great strides in all three areas, due also to a matching *TX state TRIP supplement, all of which is being used to support the Welch research project*. As per the proposal, we have already completed SG calculations of P₂O, CH₃N, and CH₃CN. The latter system (acetonitrile) is one of the largest (12D) ever considered for exact quantum dynamics calculations; we have extended the number of accurately computed vibrational states for this system from ~100 to ~10,000—an unprecedented feat, leading to a *PNAS* research report (submitted). Similar calculations for the lowest 30,000-100,000 states of benzene (30D) are currently underway. Likewise, our wavefunction-free QTM work continues to garner much attention. After two high-profile invited physics seminars presented in the last year, our earlier *JCP* article—already the most read article for January 2012 (see 2012 report)—again soared to the #1 position for six straight months, garnering nearly 20,000 downloads, making it one of the most read articles in *JCP* history. A related Welch-supported *Chem. Phys.* article from 2010 also made it to the top 20 list this past spring. Finally, additional molecular applications, Ar₃ and HO₂, also led to an Editor's Choice publication in *CPL*. Over the last twelve months, Welch support has led to four new published articles and two new articles submitted or accepted, plus nine invited and three contributed oral presentations (four international), as well as two scientific posters.

PATRICK RYAN POTTS, I-1821, The University of Texas Southwestern Medical Center. THERAPEUTIC TARGETING OF MELANOMA ANTIGEN (MAGE) GENES.

We have made significant progress on validating the MAGE-A-TRIM28 ubiquitin ligase complex as a target for anti-cancer therapeutics. We have determined that MAGE-A6, which is aberrantly expressed in cancer, is a potent oncogene that can transform normal human colonic epithelial cells. The activity of MAGE-A6 is comparable to that of expressing mutant K-Ras^{v12}, knockdown of p53, or expression of mutant Apc^{min}. We have gone on to identify the molecular mechanisms by which MAGE-A6 and the E3 ubiquitin ligase it binds, TRIM28, promote transformation of normal cells. Through proteomic arrays that contain >9,000 recombinant proteins, we identified targets of the MAGE-A6-TRIM28 E3 ubiquitin ligase complex *in vitro*. 46 targets were identified, with the AMP activated kinase (AMPK) alpha subunit being one of the top hits. AMPK is a key, central energy sensing and metabolic regulator of cells. When energy levels drop, AMPK suppresses anabolic pathways (i.e. protein and fatty acid synthesis) and promotes catabolic pathways (i.e. fatty acid oxidation and autophagy). Importantly, AMPK has been shown to be a tumor suppressor and the LKB1 activator AMPK is frequently mutated in cancer. Thus the idea that MAGE-A6-TRIM28 targets AMPK for ubiquitination and proteasomal-dependent degradation was an attractive model for MAGE-A6 oncogenic function. Biochemical and cellular studies confirmed MAGE-A6-TRIM28 regulates AMPK protein levels through ubiquitination and as a consequence regulates cellular autophagy levels, mTOR activity, fatty acid synthesis, and glucose metabolism. Finally, rescuing AMPK activity blocked MAGE-A6-induced cellular transformation. These findings validate MAGE-A6-TRIM28 as a therapeutic target and thus we have begun optimizing our biochemical alpha-screen for identifying chemical inhibitors of MAGE-A6-TRIM28. These mechanistic studies will be submitted for publication soon.

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

During 2013-2014, *we have made exciting progress in the proposed aims*. 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, we have made a novel discovery that the non-structural protein NSP2 exists in two distinct forms to coordinate the formation of the viroplasm, which are exclusive sites for virus replication (Criglar et al., 2014). Using peptide array, isothermal calorimetry, and bioluminescence interferometry we have probed into various protein-protein interactions that regulate viroplasm formation and hypothesized that NSP2 is the master regulator of the complex network of interactions that underlie viroplasm formation and genome replication (Viskowska et al. submitted). Another exciting discovery from our crystallographic studies is that the coiled-coil domain of rotavirus enterotoxin NSP4, implicated in a variety of junctions during replication, undergoes a reversible tetramer-pentamer transformation in response to changes in pH and calcium concentration (Sastry et al., submitted). In

regard to noroviruses, based on our previous crystallographic studies of protease-substrate interactions, we have made a significant and exciting progress in the synthesis and characterization of novel protease inhibitors (Deng et al., 2013). Further structure-based refinement of designing and synthesizing inhibitors that can be effective across different norovirus strains is in progress. By carrying out extensive crystallographic studies we provided a detailed structural basis for the strain-dependent glycan specificity in genogroup 1 noroviruses (Shanker et al. 2014). In regard to NS1 of influenza viruses, we have completed detailed crystallographic and biochemical studies to show that NS1, which antagonizes host antiviral responses, displays strain-dependent structural polymorphism (Carrillo et al., 2014). Further studies of how this structural polymorphism impacts NS1 interactions with various cellular proteins during virus replication is currently in progress.

HAN PU, C-1669, Rice University. EXOTIC MOLECULES FROM SPIN-ORBIT COUPLED ULTRACOLD ATOMS.

Our research has primarily been focused on the theoretical investigation of the properties of ultracold atoms and molecules. Over the past year, our main focus lies in the effects of the spin-orbit coupling in ultracold atoms induced by Raman laser fields. Such spin-orbit coupling greatly modifies the single particle density of states and, as a consequence, has a significant effect on the formation of molecular dimers from these cold atoms. We have found that in certain parameter regimes, the di-atomic molecules formed by spin-orbit coupled atoms have their lowest energy when possessing finite momentum. We are interested in calculating experimental signatures of such exotic molecules that may serve as an important guide to current experiments. In collaborating with an experimental group, we also calculated the radio-frequency spectrum of such a system. The RF spectroscopy is a well-established method in obtaining information about ultracold molecules.

FLORANTE A. QUIOCHO, Q-0581, Baylor College of Medicine. STRUCTURE-FUNCTION RELATIONSHIPS IN PROTEINS.

Inorganic phosphate (Pi) is an essential molecule for all organisms. It is required for energy metabolism, signal transduction, and biosynthesis of many diverse cellular and biochemical components. All life forms have evolved highly specific transport mechanisms to translocate the highly charged phosphate across the membrane. To fully understand Pi transport specificity, we have initiated neutron diffraction studies of the phosphate-binding protein (PBP), the initial/major Pi receptor for bacterial ATP binding cassette (ABC) phosphate transport system. Our prior x-ray diffraction atomic structures of the Pi-loaded PBP showed that the Pi is completely fully sequestered in a deep cleft, desolvated and, by inference, bound by thirteen hydrogen bonds, twelve with protein NH and OH donor groups and one carboxylate acceptor group. The carboxylate plays a key recognition role by accepting a hydrogen bond donor from either the monobasic (H_2PO_4^-) or dibasic (HPO_4^{2-}) phosphate specie. PBR phosphate affinity is relatively consistent across a broad pH range, indicating the capacity to bind both Pi species, a crucial feature extremely advantageous for cell survival especially in limiting Pi conditions or starvation. However, the mechanism by which it might accommodate the second hydrogen of monobasic phosphate is unclear. To answer this key question neutron diffraction studies were initiated. Large single crystals with a volume of 8 mm^3 were grown and subjected to hydrogen/deuterium exchange. A 2.5 \AA data set was collected at the Los Alamos Neutron Science Center. Initial refinement of the neutron data shows significant nuclear density and refinement is ongoing. This is the first report of a neutron diffraction study of a component of an ABC transporter.

ARUN RADHAKRISHNAN, I-1793, The University of Texas Southwestern Medical Center. FLUORESCENT SENSORS FOR MEASURING CHOLESTEROL IN LIVE CELLS.

In the previous year, we developed a labeled version of PFO, a bacterial protein that binds to cholesterol in cell membranes with the same specificity and sensitivity as eukaryotic cholesterol sensors, as a tool to probe cholesterol in the plasma membrane (PM) of human cells (published in the journal *PNAS*). In the current grant year, we extended the use of this tool to answer a fundamental question in cholesterol cell biology. When human fibroblasts take up plasma low density lipoprotein (LDL), its cholesterol is liberated in lysosomes and eventually reaches the endoplasmic reticulum (ER) where it inhibits cholesterol synthesis by blocking activation of SREBPs. This feedback protects against cholesterol overaccumulation in the plasma membrane (PM). But how does ER know whether PM is saturated with cholesterol? Using our cholesterol sensor, we defined three pools of PM cholesterol: 1) a pool accessible to bind PFO; 2) a sphingomyelin(SM)-sequestered pool that binds PFO only after SM is destroyed by sphingomyelinase; and 3) a residual pool that does not bind PFO even after sphingomyelinase treatment. When LDL-derived cholesterol leaves lysosomes, it expands PM's PFO-accessible pool and, after a short lag, it also increases the ER's PFO-accessible regulatory pool. This regulatory mechanism allows cells to ensure optimal cholesterol levels in PM while avoiding cholesterol overaccumulation. This work has just been published in the journal *eLife*. In the coming year, we will use fluorescently labeled sensors to study the kinetics of intracellular cholesterol transport.

MARK G. RAIZEN, F-1258, The University of Texas at Austin. STUDY OF MOLECULAR FLUIDS AND MACROSCOPIC QUANTUM PHENOMENA WITH OPTICAL TWEEZERS.

In the past year we completed a series of measurements of short-time Brownian motion in molecular fluids. We observed the instantaneous velocity of Brownian particles in liquids, predicted by Albert Einstein in 1907, although he said the experiment was impossible. This result was published in *Science* in March 2014, a follow-up on our earlier paper in *Science* from 2010 where we measured the instantaneous velocity in air. The behavior of liquids is much more complex and interesting than air. We observe memory loss, an anti-correlated thermal force, and energy equipartition. We are now improving the statistics to perform the first precision test of the equipartition theorem for a liquid. In parallel, we have set up a new system to interrogate Brownian motion on sub-nanosecond time scales, both in equilibrium and far from equilibrium. In a parallel development, we have solved the longstanding goal of nanoscale imaging of atoms. We have developed an aberration-corrected pulsed magnetic lens that will be used with a pulsed supersonic beam. This will enable the creation of

nanoscale patterns with a resolution below 5 nm. It will also be used as a chemically sensitive microscope that can probe surfaces with nanoscale resolution. In the past year we built and tested a magnetic mirror to deflect the atomic beam, and have constructed the magnetic lens.

RAMA RANGANATHAN, I-1366, The University of Texas Southwestern Medical Center. STRUCTURAL PRINCIPLES OF PROTEIN ROBUSTNESS AND EVOLVABILITY.

In our past work, we discovered a general architecture for proteins in which the central constraints on folding and function are hierarchically contained within sparse networks of amino acids (called sectors") that connect the active site to several distantly positioned surface sites. This finding provides a hypothesis for how proteins can be simultaneously robust (tolerant to mutation) and evolvable (capable of new function) - important but yet mysterious properties of proteins. The idea is that loading functional constraints within the sector permits rapid evolution of new function through variation within the sector, and yet general robustness to variation outside the sector. We set out to test this assertion through novel next-generation sequencing based methods for comprehensive mutagenesis, using two model systems - the PDZ class of protein interaction modules and the TEM-1 β -lactamase enzyme that confers bacterial resistance to antibiotics (Aim 1). This work confirms the sector hypothesis and is reported in two publications (McLaughlin et al. *Nature* 491: 138 and Stiffler et al., *Cell*, in review). In the past year, we completed Aims two and three as well, which involve a large-scale crystallographic study to mechanistically reveal how protein structures are evolved to permit adaption to new function. The data show that mutations at certain amino acid positions (largely within the sector) have the special characteristic of neutrality with regard to the current function (that is, robust), but simultaneously capable of opening up new chemical functions. Such mutations are called 'conditionally neutral', and have been theoretically proposed to be critical for the evolution of biological systems. A paper reporting these observations has now been submitted for publication (Raman et al., *Nature*, in review). These data provide the clearest evidence that the sector architecture not only supports the folding and biochemical function of proteins, but also facilitates the evolution of new functions as conditions of fitness randomly change.

HAI RAO, AQ-1747, The University of Texas Health Science Center at San Antonio. THE LAST LEG OF p53'S JOURNEY TO DEATH CHAMBER.

Recently, we demonstrate XPC as a novel regulator of p53 turnover. XPC was previously known as a key DNA repair factor. Our recent data establish XPC as a key player in proteolysis and further suggest that XPC directly binds to the Ub ligase Mdm2, which facilitates the transferring of ubiquitylated p53 to the proteasome. We have established a unique angle to understand the elusive proteasome delivery process for p53. We will further dissect the molecular and biochemical mechanisms underlying the role of XPC in p53 regulation.

The components of the ubiquitin/proteasome system are attractive drug targets, as illustrated with the efficacy of some proteasome inhibitors in the treatment of blood cancers albeit with some side effects. Since XPC regulates a subset of proteolysis and exhibits more substrate selectivity than the proteasome, XPC is likely a better drug target with less adverse effects. Identification of XPC as a novel p53 regulator presents a means to manipulate p53 level and function. Our study would not only elucidate the mechanism of XPC-facilitated p53 turnover, but also aid the search for novel strategies to boost p53 activity in cancer therapy.

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

In bacteria, 3',5'-adenosine bisphosphate (pAp) is generated from 3'-phosphoadenosine-5'-phosphosulfate in the sulfate assimilation pathway, and from coenzyme A (CoASH) by the transfer of the phosphopantetheine group to the acyl-carrier protein. We discovered a group of enzymes of unknown function that are capable of hydrolyzing pAp phosphate and AMP. Crystal structures of Cv1693 from *Chromobacterium violaceum* were determined to a resolution of 1.9 Å with AMP and orthophosphate bound in the active site. The enzyme has a trinuclear metal center in the active site with three Mn^{2+} ions. Cv1693 belongs to the Cluster of Orthologous Groups cog0613 from the polymerase and histidinol phosphatase family of enzymes. The values of k_{cat} and k_{cat}/K_m for the hydrolysis of pAp are $22 s^{-1}$ and $1.4 \times 10^6 M^{-1} s^{-1}$, respectively. The enzyme is promiscuous and is able to hydrolyze other 3',5'-bisphosphonucleotides (pGp, pCp, pUp, and pIp) and 2'-deoxy nucleotides with comparable catalytic efficiency. Enzymes from two other enzyme families have previously been found to hydrolyze pAp at physiologically significant rates. These enzymes include CysQ from *Escherichia coli* and Ytql/NrnA from *Bacillus subtilis*.

ASOK K. RAY, Y-1525, The University of Texas at Arlington. A DENSITY FUNCTIONAL STUDY OF THE SURFACE ELECTRONIC BEHAVIOR OF ACTINIDE METALS.

During the current year we have completed the following studies: (a) Atomic H interaction with the γ -U (100) surface; (b) gallium stabilized δ -plutonium alloys and hydrogen-vacancy complexes; (c) Surface properties of uranium dioxide from first principles. As a first example, theoretical analysis of H atom adsorption on the (100) surface of bcc γ -U indicates an exothermic reaction with the bridge site as the preferred site at the relativistic level of theory with spin-orbit coupling (SOC). The ground state magnetic configuration of the U-H system is found to be nonmagnetic, in agreement with experimental results for UH_3 . The change in work function of the slab with the addition of the H atom is at a maximum when the adatom is bound to the top site. H bound to the lattice in interstitial regions was also found to be exothermic in nature with the interstitial bridge site being the most stable and nonmagnetic. As a second example, All-electron density functional theory was used to investigate δ -plutonium (δ -Pu) alloyed with gallium (Ga) impurities at 3.125, 6.25, 9.375 atomic (at)% Ga concentrations. The results indicated that the lowest energy structure is anti-ferromagnetic, independent of the Ga concentration. The results also showed that the lattice constant contracts with increasing Ga concentration, which is in agreement with experimental data. Finally, all-electron hybrid density

functional theory, including spin-orbit coupling effects, has been used to study the evolution of the work function, surface energy, incremental energy, and band gap of the clean (1 1 0) and (1 1 1) surfaces of UO_2 with respect to the system size. It has been shown here that, the localization of the $5f$ electron states is pronounced at the top surface layer while bulk-like behavior is exhibited at and below the subsurface layer. The Mott-Hubbard type insulating behavior in the bulk is retained in the surfaces, albeit with a smaller band gap.

JOSEPH M. READY, I-1612, The University of Texas Southwestern Medical Center. CATALYTIC SYNTHESIS AND APPLICATION OF SUBSTITUTED YNOL ETHERS..

Our first objective was to design a synthesis of ynol ethers and ketenes. Both of these are reactive species, and thus can be converted to a variety of value-added products. To this end, we invented a Pd-catalyzed process that couples an aryl iodide with tert-butoxyacetylene ($\text{tBuO-C}\equiv\text{C-H}$). This transformation provides aryl ynol ethers ($\text{tBuO-C}\equiv\text{C-Ar}$). We showed that this reaction works with a wide variety of aryl iodides including electron-rich and electron-poor substrates. Similarly, it can be extended to include heteroaryl iodides. These reactive species can be hydrolyzed to give a variety of carboxylic acid derivatives. More interestingly, they can be converted into aryl ketenes upon heating. This process gives a very reactive reagent that can be trapped with a variety of nucleophiles. Accordingly, related to our second objective, we explored the types of reactions in which these ketenes could participate. We demonstrated that this intermediate could be converted into esters, carboxylic acids, amides, thioesters, and ketones. Thus the same intermediate gives access to a wide variety of substructures that appear in pharmaceutical agents and natural products. This work is currently in press at *Angewandte Chemie*.

With access to ynols and ketenes, we have been further exploring their reactivity. In ongoing work, we have developed a rearrangement and a cycloaddition reaction. Specifically, we find that ynols can participate in a [3+2] dipolar cycloaddition to yield a complex bicyclic product. This process forms one new ring, two new bonds, two new stereocenters and occurs with complete control of regioselectivity and diastereoselectivity. Our future plans aim to fully explore the scope of this reaction in terms of the dipoles and ynols that will participate. In a concurrent study, we have found that particular types of ketenes can undergo a coupling-rearrangement sequence to form substituted naphthalenes. Specifically, aromatic rings featuring a ketene and olefin on adjacent carbons can undergo olefination with Wittig reagents. The product allenes can then undergo a [3,3]-electrocyclic ring closure to yield, after tautomerization, the naphthalene ring. Future work aims to explore this reaction's scope as well.

LINDA E. REICHL, F-1051, The University of Texas at Austin. RELAXATION PROCESSES IN SMALL MOLECULES AND QUANTUM COHERENT SYSTEMS.

1. We have determined the lifetimes of sound modes (density waves and temperature waves) in dilute Bose-Einstein condensates. The sound mode speeds undergo an avoided crossing at very low temperature. The sound modes decay at very different rates, except in the neighborhood of the avoided crossing, where the identity of the longest-lived mode switches. Our theoretical predictions are consistent with a recent experiment on sound in a rubidium Bose-Einstein condensate.

2. The classical nonlinear dynamics of a dilute gas of rubidium atoms on a 2D optical lattice was studied for a range of polarizations of laser beams that form the lattice. We find that the dynamics ranges from integrable to chaotic as the polarizations are changed, and we describe the mechanism leading to this dramatic change in the dynamics of the gas.

3. We demonstrate that the lifetime's quasibound states in the continuum of a 1D quantum wire with two impurities, and in the presence of an electromagnetic field, can be tuned into bound states in the continuum (BIC) by changing the frequency of the radiation field. Evidence for the existence of the BIC can be obtained by observing the absorption rate of a probe photon.

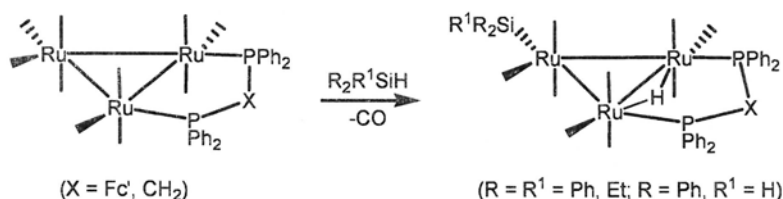
PENGYU REN, F-1691, The University of Texas at Austin. MULTISCALE MODELING OF RNA 3D STRUCTURE.

We continued to investigate the coarse-grained physical model for RNA 3D structure prediction and folding simulation. In our model, each nucleotide is represented by five coarse-grained particles. The interactions between the particles were obtained from structural statistics sampled from the experimental RNA structures in Protein Data Bank. Our coarse-grained model is unique in that it explicitly incorporates electrostatic interactions and thus responds to ionic environment, three particles are used to represent the base rings so that the stacking and pairing can be captured accurately, can be easily converted to all-atom resolution, and provides dynamics and pathway about the folding process. The model is implemented in a publicly available molecular modeling package TINKER so that other researchers will be able to utilize it. We are working to improve the accuracy of the model by refining the parameters using the experimental stability (free energy) of small duplexes. We have been improving the parallel efficiency of molecular dynamic simulations and introducing molecular-dynamics based advanced sampling algorithms (e.g. orthogonal space random walk) into TINKER. These improvements are critical to the application of the coarse-grained model toward high-throughput prediction of RNA folding, with or without (experimental) constraints. Meanwhile, we continue to make progress in understanding the principles of intermolecular forces in nucleic acids and proteins by using *ab initio* quantum mechanical methods to examine the detailed interactions of biomolecular fragments. Such understanding will enable us to develop next-generation classical physical models at both atomic and coarse-grained level for studying biomolecular structures and functions.

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

Reactions of $\text{Ru}_3(\text{CO})_{10}(\mu\text{-dppf})$ (**1**), $\text{Ru}_3(\text{CO})_{10}(\mu\text{-dppm})$ (**2**), and the ortho-metalated derivative $\text{Ru}_3(\text{CO})_9\{\mu_3\text{-PPhCH}_2\text{PPh}(\text{C}_6\text{H}_4)\}$ (**3**) with silanes (Ph_3SiH , Et_3SiH , Ph_2SiH_2) were investigated. Treatment of **1** with Ph_3SiH and Ph_2SiH_2 at room temperature leads to facile Si-H bond activation to

afford $\text{HRu}_3(\text{CO})_9(\mu\text{-dppf})(\text{SiPh}_3)$ (**4**) and $\text{HRu}_3(\text{CO})_9(\mu\text{-dppf})(\text{SiPh}_2\text{H})$ (**6**), respectively. The reaction of **1** with Ph_3SiH has been investigated by electronic structure calculations, and these data have facilitated the analysis of the potential energy surface leading to **4**. Compound **1** does not react with Et_3SiH at room temperature but reacts in refluxing hexane to give $\text{HRu}_3(\text{CO})_9(\mu\text{-dppf})(\text{SiEt}_3)$ (**5**) in good yield. Reaction of **2** with Ph_3SiH at room temperature yields two new products: $\text{HRu}_3(\text{CO})_9(\mu\text{-dppm})(\text{SiPh}_3)$ (**7**) and $\text{H}_3\text{Ru}_3(\text{CO})_6(\mu_3\text{-O})(\mu\text{-dppm})(\text{SiPh}_3)$ (**8**), with the latter formed as minor by-product due to the presence of adventitious water. At room temperature compound **7** slowly reverts back to **2** in solution with decomposition and liberation of Ph_3SiH . Similar reactions of cluster **2** with Et_3SiH and Ph_2SiH_2 give only intractable materials. The ortho-metalated cluster **3** does not react with Ph_3SiH , Et_3SiH and Ph_2SiH_2 at room temperature but does react at elevated temperature to give $\text{HRu}_3(\mu\text{-CO})(\text{CO})_7\{\mu_3\text{-PPhCH}_2\text{PPh}(\text{C}_6\text{H}_4)\}(\text{SiR}_2\text{R}^1)$ (**9**, $\text{R} = \text{R}^1 = \text{Ph}$, 71% yield; **10**, $\text{R} = \text{R}^1 = \text{Et}$, 60% yield; **11**, $\text{R} = \text{Ph}$, $\text{R}^1 = \text{H}$, 66% yield) by activation of the Si-H bond. The solid-state structures of clusters **4** and **8-11** have been determined by X-ray crystallography. In **4**, both the dppf and the hydride bridge a common Ru-Ru vector, whereas NMR studies on **7** indicate that two ligands span different Ru-Ru edges. Compound **8** contains a face-capping oxo moiety, a terminally coordinated SiPh_3 ligand, and three bridging hydride ligands, whereas **9-11** represent simple oxidative addition products. In all of the clusters examined, the triruthenium framework retains its integrity and the silyl groups occupy equatorial sites.



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

The second year of this project supported two graduate students and resulted in five published articles, two submitted manuscripts, and one provisional patent. Research on calcium oxalate monohydrate (COM) crystallization led to the successful identification of natural promoters of crystal growth, which is a rare occurrence in biomineralization. Typically modifiers act as inhibitors, but we discovered two cationic proteins interact with COM surfaces and promote the kinetic rate of crystal growth. More interesting is the fact that the mechanism differs from other promoters identified in literature. We worked with the Karande Group at Rensselaer Polytechnic Institute to synthesize and test peptide segments of the most effective promoter, lysozyme. Our studies reveal that this protein is comprised of individual sequences that act either as a promoter or an inhibitor of COM growth. This work was submitted for publication in *JACS*. We have extended this research to studies of β -hematin crystallization, which is the byproduct of malaria. We are interested in examining the specific interactions of antimalarial drug molecules with β -hematin crystal surfaces. The groundwork for this project involved the quantification of critical thermodynamic parameters (e.g., hematin solubility), the design of a biomimetic growth solution, and the synthesis of large crystals amenable for AFM studies. We succeeded in these tasks and published two manuscripts. We also made significant advancements with *in situ* AFM studies of β -hematin surface growth, which is now being prepared as a manuscript. A major breakthrough in this project was the design of a unique liquid AFM cell that permits time-resolved imaging of crystal growth at high temperature. Until now, AFM measurements have been limited to low temperature and short times. We circumvented this problem and selected the mineral silicalite-1 to test the new system. Continuous imaging at 80 °C for 24 hours provided evidence of the silicalite-1 growth mechanism, which occurs by both classical and non-classical pathways. This was the first *in situ* measurement of silicalite-1 growth, and establishes a platform for studies of other materials that grow in solvothermal conditions (e.g., metal oxides and MOFs). This landmark work was published in *Science Magazine*.

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

Complexins are small soluble proteins that play both activating and inhibitory roles in neurotransmitter release through its various domains, which include a central helix that is crucial for all complexin functions and an accessory helix that inhibits release. A widely accepted model proposed that this inhibitory role arises because the accessory helix inserts into partially assembled SNARE complexes that bridge the synaptic vesicle and plasma membranes before calcium triggers release. This model was supported by a so-called superclamp mutation that replaced three charged residues with hydrophobic residues and enhanced the inhibitory activity of complexin in cell-cell fusion assays, as well as by the decreased inhibition observed in these assays for a poor-clamp mutant and by a crystal structure obtained with a superclamp mutant and a synaptobrevin-truncated SNARE complex. We have performed an extensive analysis by NMR spectroscopy and isothermal titration calorimetry that shows that the complexin accessory helix does not insert into synaptobrevin- or syntaxin-truncated SNARE complexes in solution. Moreover, we found that the complexin superclamp mutant has slightly activating or no effects on neurotransmitter release *in vivo*, while the poor-clamp mutation inhibits release. Importantly, we showed that increasing or decreasing the negative charge of the accessory helix decreases or increases release, respectively. These results suggest a novel model whereby the accessory helix inhibits release through electrostatic interactions with the synaptic vesicle and plasma membranes. We have also completed a study describing the structure and calcium binding properties of extended synaptotagmin 2.

JON D. ROBERTUS, F-1225, The University of Texas at Austin. MECHANISM OF FOLATE-DEPENDENT METHYLATION.

We made a major breakthrough this past year in the analysis of fungal Met6p. Several structures of cobalamin-independent methionine synthases have been solved. The protein is large, with two 13-barrel domains; the homocysteine (Hcy) substrate is bound deep in the C-terminal barrel, and the 5-methyl tetrahydrofolate (5Me-THE)1 substrate is bound largely in the N-terminal domain. In all cases to date the structures are in an OPEN configuration; that is the two domains are separated and the substrates cannot interact. It has been inferred that Met6p must undergo a major conformational change to close up the active site. This year we were able to solve the X-ray structure of a closed form with both substrates bound. We showed that the closure involves a rigid body rotation of the N-terminal barrel of about 12° around an axis along with the concomitant rearrangement of a key surface loop in the C-terminal barrel. Our structure also shed light on this interesting chemical reaction. The cobalamin-independent methyl transfer has been puzzling, since the Hcy thiol is a modest nucleophile and the THE group is a very poor leaving group. We have shown, by X-ray crystallography and site directed mutagenesis, that His707 (via a bound water molecule) protonates the leaving THF at N5 to facilitate the reaction.

DANIEL ROMO, A-1280, Texas A&M University. NOVEL STRATEGIES FOR BIOACTIVE NATURAL PRODUCT SYNTHESIS VIA β -LACTONE INTERMEDIATES AND NEW METHODOLOGY FOR ASYMMETRIC ALKYLATIONS.

In this past grant period, we started to fully explore the great potential of chiral, unsaturated acylammonium salts that are readily accessible from a number of commercially available, commodity unsaturated acid chlorides and isothiouraea catalysts. To date, we have demonstrated the utility of these intermediates in a number of organocascade processes including a nucleophile(Lewis base)-catalyzed Michael-aldol- β -lactonization cascade (NCMAL), a Michael-Michael-aldol- β -lactonization (MMAL), a Michael-proton transfer- γ - and δ -lactamization, and most recently a Diels-Alder- γ - and δ -lactonization (DAL). We are currently exploiting the versatility of these developed synthetic methodologies toward a number of bioactive natural products that will form the basis of detailed mechanistic studies of their mode of action. In addition, we are studying the full potential of chiral unsaturated acylammonium salts for both asymmetric carbocycle and heterocycle synthesis.

MICHAEL J. ROSE, F-1822, The University of Texas at Austin. LIGATION OF HEAVY ATOM DONORS TO FIRST ROW TRANSITION METALS.

We have made significant progress in assembling the heavy-atom containing ligands. Our work thus far has focused on the intermediate weight donor atom in the series As→Sb→Bi. Antimony chemistry is quite unlike that of its lighter analog, phosphorous, and we are implementing known synthetic methods as well as developing new approaches. We have prepared the target ligand {Me[Sb(Ph)₂]₃}, and we are preparing {Me[Sb(Pr)₂]₃} and {Ph[Sb(Pr)₂]₃} to exhibit enhanced stability under metalation conditions. Consistent with others' findings, we have found that the Sb-phenyl bond is readily broken under mild synthetic or metalation conditions. We have also discovered a novel di-antimony containing ligand based on a naphthalene scaffold [(Naphth)₂•1,8-antimide]. The ligand will act as a chelating Sb₂ ligand, and may exhibit redox activity (making and breaking the Sb-Sb bond) to enhance catalysis. Preliminary ligation studies with Sb-containing ligands indicate that reactions with first row metals are quite different than phosphorous chemistry, and that choice of solvent (non-coordinating) and metal oxidation state (-2→1) are critical variables.

The grant has supplemented exploratory research into activation of CO₂ and O₂ with first row metals. We have developed a CO₂ reduction catalyst based on a diglyoxime-naphthalene unit that acts as a multi-electron reservoir during the 2e⁻/2H⁺ reduction of CO₂ to CO. In separate work, we have discovered an auto-dinucleating di-cobalt system derived from an N4 ligand that captures O₂ in a stable dicobalt(III)/ μ -peroxo adduct. This adduct resembles a critical intermediate step in water oxidation – a fundamental reaction to develop a Solar Fuels based, carbon-free fuel cycle.

MICHAEL K. ROSEN, I-1544, The University of Texas Southwestern Medical Center. PHASE TRANSITIONS IN MULTIVALENT MACROMOLECULAR ASSEMBLY.

We have found that the electrostatic properties of the linker connecting the first and second SH3 domains of Nck substantially influence the ability of Nck to drive phase separation in the pNephrin/Nck/N-WASP system. The natural linker consists of an N-terminal basic region and a C-terminal acidic region. Replacement of this sequence with a generic unfolded sequence increases the critical concentration for phase separation in both 3D and 2D systems, and also decreases the weak ability of Nck to self associate (indicated by a change in the second virial coefficient). Shuffling the charged residues to eliminate the segregation in the natural sequence (but maintaining overall amino acid composition) has the same effects. Importantly, a shuffle that enhances the charge separation, has the opposite effect. These data suggest that charge separation in disordered linker regions of adaptor proteins may be generally important to their ability to self-associate and promote phase separation. We have also shown that increasing the affinity of Nck for pNephrin decreases the dynamics of all components of the clusters, again suggesting a general relationship between module-module interactions and properties of phase separated clusters. Finally, we have found that pNephrin/Nck/N-WASP clusters potently assemble actin filament networks through the Arp2/3 complex, likely through the increase in N-WASP density that occurs upon clustering.

DANIEL M. ROSENBAUM, I-1770, The University of Texas Southwestern Medical Center. STABILIZATION OF ACTIVE AND INACTIVE CONFORMATIONS OF OREXIN RECEPTORS FOR CRYSTALLIZATION.

My lab works on biophysical characterization of integral membrane proteins involved in cellular signaling and human disease. Over the past year of Welch Foundation support, we have been working to obtain high-resolution crystal structures of several physiologically important disease-related GPCRs. Solving GPCR structures is difficult due to problems with expression, purification, and stabilization of functional human membrane proteins. Previously I

helped pioneer the engineered fusion protein approach to GPCR crystallization, which has led directly to the structure determination of over 20 GPCRs. My lab recently expanded this approach to include new fusion protein partners, which has enabled expression and crystallization of previously inaccessible GPCR targets. This Welch Foundation grant focuses on using these protein engineering strategies to solve structures of the human orexin receptor, a CNS modulator of sleep-wake cycles in mammals whose activity is compromised in the disease narcolepsy. Whereas our previous fusion proteins were incapable of producing milligram quantities of the orexin receptor for structural biology, our new fusion proteins have quickly allowed us to express, purify, and attempt crystallization. Over the past year, we have been able to produce microcrystals of this GPCR using lipid-mediated crystallization, and we are in the process of testing these crystals for X-ray diffraction. Solving the structure of the orexin receptor will help us understand the mechanism of orexin neurotransmitters and synthetic compounds that target the receptor, and will aid in the design of more potent and selective ligands. In addition to these studies, we have been engaged in collaboration with Patrick Barth's lab at the Baylor College of Medicine, who uses computational approaches to design GPCR mutants that are stabilized in the agonist-bound active conformation. Through this collaboration, we will be able to rapidly pursue crystal structures of a number of physiologically and biomedically important GPCRs in both active and inactive conformations.

JOSEPH H. ROSS, JR., A-1526, Texas A&M University. MAGNETISM AND ANHARMONIC LATTICE VIBRATIONS IN CLATHRATES AND RELATED MATERIALS.

This year as an extension of our work on Ba-Cu-Ge clathrates, we investigated several Si analogs of these compounds, which are of recent interest as potentially inexpensive thermoelectric generator materials. Our NMR results confirm a change to gapless semiconductor behavior in $\text{Ba}_8\text{Cu}_5\text{Si}_{40}$, in agreement with recent theory. We studied new Co-substituted clathrates, $\text{Ba}_8\text{Ge}_{43-x}\text{Co}_y$ and $\text{Ba}_6\text{Ge}_{25-x}\text{Co}_x$, finding solubilities considerably less than the expected Zintl composition. Thermal and electrical transport and Ba and Co NMR measurements demonstrated a corresponding metallic behavior and allowed us to track the $\text{Ba}_6\text{Ge}_{25}$ structural transition vs. doping. Further measurements focused on BaGaGe clathrates and $\text{Yb}_x\text{Co}_3\text{Sb}_{12}$ -based skutterudites. For these investigations we developed an apparatus for Hall Effect measurement in our NMR facility, and extended capabilities for heat capacity measurement. The latter was also used for continued investigation of BaFe_2As_2 materials, demonstrating changes of the enhanced magnetic fluctuation contribution to the magnetic entropy with heavy ion substitution, and in NiMnIn compounds, with new results providing conclusive demonstration and characterization of the antiferromagnetic low-temperature structural phase coexisting with superparamagnetic clusters. We also launched a new investigation of Cu_2Se and Cu_2Te -based semiconductors, which are of much current interest for photo- and thermo-electric applications. New results include demonstration of anharmonic local-oscillations of Cu ions probed by quadrupole-NMR relaxation behavior, transitioning to incipient superionic motion well below room temperature, and also metastability associated with the high-temperature structural phase transition.

RICK RUSSELL, F-1563, The University of Texas at Austin. INVESTIGATION OF RNA MISFOLDING DURING TRANSCRIPTION.

In the past year, we continued making very rapid progress on the folding pathways and misfolding of the *Tetrahymena* ribozyme. A series of RNA mutants showed that a key native secondary structure (P3) is formed early in folding and must be broken later for folding to proceed to the native state, whereas P3 remains intact during subsequent folding to the long-lived misfolded state. The requirement for P3 to be broken implies that the incorrect topology is also formed early in folding, because its resolution apparently requires disruption of P3. Thus, the overall picture that emerges is that incorrect positioning of two domains leads to the incorrect topology forming early in folding. This topology is then stabilized by the subsequent formation of native secondary and tertiary contacts. We anticipate that this model will serve as a useful paradigm for understanding folding of larger and more complex RNAs such as the ribosomal and spliceosomal RNAs. In addition, we studied the topology of DNA junctions in collaboration with Makkuni Jayaram and we studied RNA-RNA interactions of another type of structured RNA, a group 11 intron, with the ribosome in collaboration with Lydia Contreras and Marlene Belfort.

SANDRA L. SCHMID, I-1823, The University of Texas Southwestern Medical Center. CONFORMATIONAL DYNAMICS AND REGULATION OF DYNAMIN.

We have been successful in developing fluorescence-based assays to measure conformational changes that affect interactions between dynamin's pleckstrin homology domain (PH) and its stalk. These assays have revealed that dynamin in solution exists in equilibrium between a closed (PH domain docked to the stalk) and open (PH domain no longer closely interacting with stalk) state. Membrane binding shifts dynamin to the open conformation. By introducing single cysteines in the PH domain and stalk we can crosslink dynamin, locking it in the closed conformation. Crosslinked dynamin can no longer assemble onto membranes. Interestingly, we also have data to suggest that binding of some (amphiphysin, endophilin), but not all (SNX9) SH3 domain-containing partners to dynamin's PRO shifts this equilibrium to the open state, presumably through some global conformational changes given that the PH domain and PRO are distally located. Finally, we have discovered that a disease-causing mutant of dynamin-2 (S619L), implicated in Centronuclear Myopathy (CNM) appears to be in an 'activated' conformation based on its highly enhanced basal GTPase activity, primarily exists in the closed state at 37°C, and fails to interact with lipid membranes. Nonetheless, this mutant is capable of opening up and facilitating membrane interaction at 22°C. We are currently collaborating with Patrick Griffin at Scripps Florida to perform hydrogen-deuterium exchange reactions, coupled with mass spec to identify regions involved in these global conformational changes.

J. MARTIN SCHOLTZ, BE-1281, Texas A&M University System Health Science Center. FORCES INVOLVED IN PROTEIN FOLDING AND STABILITY.

We continue to make some important advances toward an understanding of the specific details of the molecular determinants of protein stability and folding. Our current project remains focused on the forces and interactions involved in the buried parts of proteins, especially those that involved a charged or polar group. We are trying to understand how the protein interior can tolerate and accommodate polar groups buried in an otherwise unfavorable (very hydrophobic) environment. This is a very difficult experiment to accomplish because polar group burial greatly destabilizes proteins and they never fold. Our solution is to use a very stable variant of our model protein, ribonuclease Sa, such that we can introduce a polar group into the interior at a site near hydrophobic residues. We have also designed other variants in which we place polar groups near other polar groups including both backbone and side-chains. Using the three-dimensional structures of the proteins as a guide, we select residues that are buried in the interior of the protein at sites with different properties. Side-directed mutagenesis allows us to change the DNA sequence and the resulting recombinant protein is expressed and purified. This approach allows us to alter any existing amino acid and produce adequate amounts of protein for our studies.

HANS A. SCHUESSLER, A-1546, Texas A&M University. OPTICAL STUDIES OF ULTRA COLD MOLECULAR IONS USING FEMTOSECOND AND XUV LASER RADIATION.

We continued experiments on laser and sympathetically cooled fullerene ions. The trapping of ions with such different masses (C_{60}^+ , Mg^+) can be improved by using two-frequency RF fields. We developed precision broadband spectroscopic techniques with frequency combs, including Vernier spectroscopy, and as first application carried out precision measurements of the molecular spectra of the greenhouse gases CH_4 , CO and CO_2 in the IR regions. We achieved an absorption sensitivity of $\sim 8 \times 10^{-8} \text{ cm}^{-1} \text{ Hz}^{-1/2}$ corresponding to a detection limit of ~ 70 ppbv for acetylene, with a resolution of ~ 1.1 GHz. The fast data acquisition rate with dual frequency comb spectroscopy opens the way to quantify some gas phase chemical reaction rates. With femtosecond pulses and utilizing a deconvolution technique above-threshold ionization (ATI) spectra of xenon were obtained with higher contrast and are in excellent agreement with characteristic two and ten Up cutoff energies contrary to that found for raw data and simultaneously the experiment also revealed the presence of a second electron from double ionization. We obtained experimental results on the fragmentation of methane in femtosecond pulses and also investigated the angular anisotropy of photo fragmentation. We find evidence of multiple dissociation mechanisms including statistical decay, field-assisted dissociation, and Coulomb explosion. For trapped and laser cooled beryllium ions our study of the distribution of the halo neutron of the single neutron halo nucleus 11Be used the Bohr-Weisskopf effect.

MARLAN O. SCULLY, A-1261, Texas A&M University. STUDIES IN LASER AND QUANTUM CHEMISTRY.

This past year, our group has made many discoveries and advancements as relates to superradiance, surface plasmon amplification, Bohr's molecular model, high frequency lasers, and more. Highlights include:

- Development of a new kind of quantum amplifier called a QASER (Quantum Amplification by Superradiant Emission of Radiation) whose operation is based on collective superradiant emission and does not require population inversion. The QASER was found to be many orders of magnitude more efficient than the usual nonlinear multiphoton excitation and holds promise for a new kind of high-frequency coherent radiation generator.
- Investigation into surface plasmon amplification in a silver nanoparticle coupled to an externally driven three-level gain medium. We discovered that quantum coherence significantly enhances the generation of surface plasmons. Surface plasmon amplification by stimulated emission of radiation was achieved in the absence of population inversion on the spasing transition, which reduced the pump requirements. The coherent drive allowed us to control the dynamics and holds promise for quantum control of nanoplasmonic devices.
- Investigation into Bohr's century-old model and discovered that in the limit of infinite dimensions it is reconciled with quantum mechanics and yields surprisingly accurate predictions for hydrogen and other small molecules. Our results, coined as "Bohr's Molecular Model, a Century Later" were published in *Physics Today*.
- Investigation of LWI in the extreme-ultraviolet (XUV) within the context of tunable-ultrashort-high-power laser Pulses . We found that transient LWI holds promise for a different LWI paradigm in which the lasing is based on forbidden and/or virtual transitions. This yields an excellent possibility for overcoming the restrictions imposed on the decay rates associated with the usual LWI schemes when results are extended from other regimes to XUV.

LAURA SEGATORI, C-1824, Rice University, PHYSICOCHEMICAL PROPERTIES OF NANOPARTICLES AT THE INTERFACE WITH BIOLOGICAL SYSTEMS.

Most nanoparticles (NPs) enter the cells through endocytosis and are found within endosomes and lysosomes. Subsequent routing to autophagosomes was observed for a range of NPs of different material and charge. Because the composition and surface chemistry of these NPs vary significantly, the nanoscale size seems to be the common denominator for accumulation into autophagosomes and induction of autophagy. The impact of NPs on downstream steps of the autophagy pathway, however, is likely to depend on other physicochemical properties, including material and charge. We recently completed a comprehensive study aimed at elucidating the impact of 2-hydroxypropyl- β -cyclodextrin (HP β CD) on the autophagy system. We found that internalization of HP β CD results in activation of autophagy and in enhancement of the cellular autophagic clearance capacity. Interestingly, HP β CD-mediated activation of autophagy was found not to depend on the ability of HP β CD to extract cholesterol from cellular membranes. We also investigated the interface between cerium oxide NPs and the autophagy system. Cerium oxide is a rare earth metal oxide with a cubic fluorite structure that contains ceria in two different oxidation states (cerium(III) and cerium(IV)). This mixed valency confers ceria nanocrystals with interesting properties in aqueous cellular

environments in which cerium(III) reacts with reactive oxygen species and cerium(IV) reverts back to its original state. We tested a battery of ceria nanoparticles functionalized with different types of biocompatible coatings (N-Acetylglucosamine, polyethylene glycol and polyvinylpyrrolidone) expected to have minimal effect on lysosomal integrity and function. We found that ceria nanoparticles function as autophagy activators and promote clearance of autophagic material.

PHILIP SERWER, AQ-0764, The University of Texas Health Science Center at San Antonio. STRUCTURAL CHEMISTRY OF VIRUSES.

We have previously shown that DNA-containing, tail-free, bacteriophage T3 heads leak DNA in quantized amounts. The heads were originally obtained from a 5-site T3 mutant ($T3^{SR3-1}$; three tail mutations) selected for propagation in media with 0.9 M NaCl (relatively high). We have now shown that quantized leakage also occurs from heads obtained via single-site tail amber mutants. When we chelate magnesium cation, DNA leakage accelerates. The product of leakage is stable. We have used these results to develop procedures of DNA hydration-based preparative and analytical Nycodenz buoyant density centrifugation to isolate and characterize DNA packaging intermediates (called native intermediates) with some DNA packaged and some not. Density in Nycodenz gradients decreases (hydration increases) as external DNA length increases at the expense of packaged DNA. We have also developed native gel electrophoresis to rapidly identify native intermediates. Use of the above revealed that $T3^{SR3-1}$ does not accumulate native intermediates. However, in traditional medium with 0.1 M NaCl, $T3^{SR3-1}$ does dramatically accumulate intermediates (called ipDNA-capsids) with incompletely packaged DNA and no visible external DNA segment. Some ipDNA-capsids have the packaging motor, based on electron microscopy. These observations are explained by assuming that stalling of packaging occurs *in vivo* and (1) triggers DNA cleavage, (2) increases for $T3^{SR3-1}$ and (3) evolved to provide time for feedback control.

JONATHAN L. SESSLER, F-1018, The University of Texas at Austin. MOLECULAR RECOGNITION VIA BASE-PAIRING.

During this grant period the fundamental determinants behind thermal and photo-induced electron transfer (ET) within supramolecular assemblies were studied. We investigated *inter alia* the effect halide anions and their tetraalkylammonium (TAA) counter cations have on the binding of fullerenes (C_{60} and C_{70}) with tetrathiafulvalene calix[4]pyrroles (TTF-C4Ps) in solution and in solid-state. We found anions bind to the TTF-C4Ps to induce a conformational change from the 1,3-alternate to the cone conformation that resembles a cup into which fullerenes can fit in a "ball in socket" binding mode. This binding results in a charge transfer (CT) complex with 1:1 binding stoichiometry. The halides studied (F^- , Cl^- , Br^-) all induce the cone conformer of the TTF-C4P, with the strongest binding to C_{60} achieved with the smaller, more basic fluoride anion. However, in the case of the elliptical C_{70} , the largest binding affinity was attained with the larger chloride anion. In this case, the smaller fluoride anion allows for the TTF-C4P cone conformer to adopt a wider bite angle, a larger bowl radius, than chloride, which is needed to accommodate the larger, spherical C_{60} . The TAA counter cation also plays an important role in fullerene binding in that smaller cations, such as tetraethylammonium (TEA^+), can compete for the TTF-C4P cavity, displacing the fullerene and acting as an allosteric effector.

The photo-induced ET from TTF-C4P to a porphyrin carboxylate within a supramolecular ensemble was also studied in this grant period. The carboxylate moiety of the porphyrin binds to the TTF-C4P in the same manner as halide anions. Photo-irradiation of the porphyrin followed by ET from the TTF-C4P to the porphyrin produces the TTF-C4P radical cation and the porphyrin radical anion. The charge-separated (CS) state produced upon photo-irradiation has one of the longest known lifetimes for a CS generated via PET in a non-covalently bound complex.

A number of other supramolecular systems were also studied.

LIBO SHAN, A-1795, Texas A&M University. BIOCHEMICAL AND REGULATORY CONSTRAINTS OF IMMUNE SENSORS.

The first line of innate immune responses is initiated by the recognition of conserved microbial signatures via membrane-resident receptors, which are often encoded by receptor-like kinases (RLKs) in plants. The dimerization and phosphorylation of receptor-like cytoplasmic kinases (RLCKs) in the receptor complex constitute essential steps to initiate immune signaling. Two *Arabidopsis* RLKs FLS2 and BAK1 interact with RLCK BIK1 to initiate and transduce plant immune responses to bacterial flagellin. BAK1 directly phosphorylates BIK1 to positively regulate plant immunity. BIK was classically defined as a serine/threonine protein kinase and many serine/threonine residues are required for BIK1 functions. We have found that BIK1 also possesses tyrosine kinase activity, is auto-phosphorylated and trans-phosphorylated by BAK1 at multiple tyrosine residues. Mutational and transgenic analyses support the vital role of tyrosine phosphorylation in BIK1-mediated plant innate immunity as certain BIK1 tyrosine mutations were no longer able to complement the *bik1* mutant plant-associated compromised immune responses. In addition we found that bacterial Type III effector HopF2 suppresses *Arabidopsis* innate immunity triggered by multiple microbe-associated molecular patterns (MAMP) by direct interaction with BAK1 at the plasma membrane.

JASON B. SHEAR, F-1331, The University of Texas at Austin. CREATING 3D CELL CULTURES USING MULTIPHOTON PHOTOFABRICATION WITH DYNAMIC ELECTRONIC MASKS.

With the Whiteley group at UT Austin, we investigated O_2 availability within biologically relevant, micrometer-scale bacterial aggregates since oxygen concentration impacts a number of important bacterial processes. *P. aeruginosa* were confined within gelatin-based 3D microtraps of varying sizes and geometries, and using a GEP-reporting system responsive to cellular O_2 levels, showed that as a single bacterium grows into a maximally dense clonal population, a local depletion of O_2 develops when it reaches a critical aggregate size, demonstrating that phenotypic heterogeneity can exist on the micrometer scale within small bacterial aggregate populations.

We continued our studies on the novel use of our 3D printed protein microforms as substrates for performing real-time modification of cell-culture surfaces, and have shown that fibroblast cells can be induced to undergo large changes in alignment and morphology by creating grooves of arbitrary dimensions and placement at select times during cellular growth. This tool for use is expected to have applications in areas such as cell motility and stem-cell

differentiation.

In a further extension, we collaborated with the Finkelstein lab at UT Austin to use our 3D printing technology to study replicative cellular aging, using the yeast, *S. pombe*, as a relevant model. Microfluidic systems were designed and rapidly prototyped to create devices capable of capturing yeast cells suspended in media. By continuously removing progeny cells from collection sites for parent cells following cycles of division, we demonstrate that cell growth and protein aggregation can be tracked in individual cells for over ~100 h. This device provides a powerful on-chip microdissection platform that will enable high-throughput studies of aging in rod-shaped cells.

A. DEAN SHERRY, AT-0584, The University of Texas at Dallas. LANTHANIDE-BASED CEST AGENTS FOR MOLECULAR IMAGING.

The rate at which water molecules exchange between an inner-sphere water coordination position in a paramagnetic lanthanide complex and bulk solvent is a key parameter for the design of optimal functional MRI contrast agents. The measurement of water exchange rates by ^{17}O NMR and other water proton linewidth measures has been provided new insights into three different classes of MRI contrast agents, those based on changes in the T_1 of water protons, those based on T_2 or apparent T_2 due to chemical exchange ($T_{2\text{exch}}$), and those based on chemical exchange saturation transfer (CEST). The relationships between the chemical structure of the ligands used to encapsulate a lanthanide ion and the measured water exchange rates now allow us to design complexes that display water exchange rates that vary over six orders of magnitude. Those insights allowed us to develop a more sensitive T_1 agent for detection of Zn^{2+} ions released by pancreatic beta cells in response to high glucose and for detection of Zn^{2+} ions in healthy prostate tissues in animals *in vivo*. Complexes having an water exchange rate for providing the most sensitive $T_{2\text{exch}}$ contrast have also been identified, and for providing the most sensitive CEST agents for imaging important tissue parameters such as pH, reactive oxygen species (ROS) and hypoxia have been identified. Our long-term goal is to build platform technologies that will allow direct imaging of these various physiological parameters *in vivo* by MRI. Thus, the basic studies support by this grant continue to impact our ability to create new MRI contrast agents for monitoring metabolism and physiology *in vivo*.

XIAOBING SHI, G-1719, The University of Texas M. D. Anderson Cancer Center. MOLECULAR MECHANISMS OF JARID1B PHD FINGERS IN RECOGNITION OF HISTONE METHYLATION.

In the past year, we have made several progresses as outlined below:

1. In collaboration with Dr. Tatiana Kutateladze from University of Colorado Denver, we solved the NMR structure of the PHD1 and PHD3 of JARID1B. In collaboration with Dr. Wei Li's lab at Baylor, we performed RNA-seq analysis in JARID1B knockdown cells and identified JARID1B target genes in the triple negative breast cancer MDA-MB231 cells genome-wide. We also generated stable MDA-MB231 cells expressing WT, PHD3 (H3K4me3-binding deficient) and PHD1 (H3-binding deficient) mutants, which provided us a tool to overcome the difficulty we had in the past two years for chromatin IP (due to the lack of ChIP-grade antibody). Using Flag antibody, we are able to ChIP down both WT and mutant JARID1B in cells. We also performed a number of functional analyses in control and knockdown cells to determine the role of JARID1B in cell growth, cell migration and invasion. Together, we published our findings in *Cell Reports* this year.

2. We have two other papers, including one paper on *Nature*, published the past fiscal year that are partially supported by the Welch grant.

CHIH-KANG SHIH, F-1672, The University of Texas at Austin. QUANTUM CONTROL OF LIGHT-MATTER INTERACTIONS IN METALLIC QUANTUM STRUCTURES.

In this grant reporting period, our research work was focused on:

- Probing the intrinsic optical constants of epitaxial thin Ag films on Si(111) and carrying out direct measurement of the surface plasmon polariton (SPP) propagation length as a function of the optical wavelength and the other materials parameters such as surface roughness (in collaboration with Professor Xiaojin Li' manuscript accepted for publication in *Advanced Materials*)

- Demonstration of All color plasmonic nanolaser on a single materials platform (manuscript accepted for publication in *Nano Letters*)
Manipulating the plasmonic enhanced upconversion of NaYF_4 fluorescent nanoparticles through precise tuning of plasmonic resonances. (Manuscript under preparation)

- In addition to these research activities directly relevant to the original research scope, the Welch supports further allow us to venture into other activities enabled by the capability to grow epitaxial thin metal films as well as 2D monolayer materials. These results have been published in several journals.

OK-HO SHIN, H-1771, The University of Texas Medical Branch at Galveston. KINETICS AND EQUILIBRIA OF THE SNARE COMPLEX ASSEMBLY.

Cpx or Munc18 potentiates the SNARE-mediated exocytotic process in neuronal cells. Therefore, these proteins are probably involved in promoting the assembly of SNARE complex formation. To test the hypothesis, we measured efficiencies of the syntaxin 1B/SNAP25/syntaxin1B complex formation in the presence of Cpx and/or Munc18 by employing a yeast four (syntaxin1B, SNAP25, syntaxin1B, and either Cpx 01 Munc18)- or five (syntaxin1B, SNAP25, syntaxin1B, Cpx, and Munc18)-hybrid interaction assay. In a yeast four-hybrid interaction assay, either Cpx or Munc18 strongly inhibited the formation of syntaxin1B/SNAP25/syntaxin1B complex due to the formation of Cpx/syntaxin1B/SNAP25 complex or Munc18/syntaxin1B complex. We determined whether the presence of both Cpx and Munc18 ameliorates the inhibitory effect of either Cpx or Munc18 alone by employing a yeast five-hybrid assay. In the presence of both Cpx and Munc18, the efficiency of syntaxin1B/SNAP25/syntaxin1B complex formation was further inhibited in an additive manner. Therefore, Cpx and Munc18 promote the SNARE-mediated exocytotic process probably in the presence of other proteins that are also involved in the

SNARE-mediated exocytosis in neuronal cells. Our results indicate that the function of Cpx and Munc18, which promote the SNARE-mediated exocytosis in the cell, cannot be investigated in an isolated interaction assay system which is composed of only SNARE proteins.

QIMIAO SI, C-1411, Rice University. THEORETICAL STUDIES OF ELECTRONIC DYNAMICS AND CORRELATIONS IN CARBON-BASED AND RELATED NANOSTRUCTURES.

During the past year, we made the following progresses:

- Electronic dynamics and correlations in graphene. We studied two models on a honeycomb lattice, which defines the structure of graphene. We analyzed the role of spin-orbit coupling, and identified novel electronic states that possess unusual electronic characteristics both in the bulk and at the boundary. One paper each appeared in *PRL* and *PRB*.

- Defects in low-dimensional systems. Reduced dimensionality often yields non-constant density of electronic states near the Fermi energy. We studied the behavior of electronic defects embedded in such a low-dimensional electronic bath. We found parameter regimes where the spins of the defects are distinctly screened by those of the bath, and determined the signatures of such effects in the spin dynamics. Two papers appeared in *FRB*.

- Quantum criticality and superconductivity due to electron correlations. We discovered a new Ni-based system in which quantum criticality can be observed. We also carried out microscopic calculations and collaborated with experimentalists to determine novel properties of superconductivity in several Fe-based systems. Five papers were published, including one in *Nature Communications* and one in *PRL*.

DIONICIO R. SIEGEL, F-1694. The University of Texas at Austin. SYNTHESIS OF REGENERATIVE NATURAL PRODUCTS.

The first biological target for the natural product complanadine A has been determined. The pseudosymmetric alkaloid functions as a selective agonist for the Mas-related C protein-coupled receptor X2 (MrgprX2), a G protein-coupled receptor that is highly expressed in neurons. Given the potential of MrgprX2 to function as a modulator of pain, complanadine A represents a new chemical probe to selectively interrogate the physiological function of MrgprX2 as well as a potential lead for the development of antihyperalgesics for the treatment of persistent pain. White complanadine A possess agonistic activity the related natural product lycodine, representing halt of complanadine A, and lacks activity providing a cursory description of the structural requirements for agonistic activity.

A general protocol for exogenous small-molecule pull-down experiments with *Caenorhabditis elegans* is described; it provides a link between small-molecule screens in worms and existing mutant and RNAi technologies, thereby enabling organismal mechanism of action studies for the natural product clovanemagnolol. Forward chemical genetic screens followed by mechanism of action studies with *C. elegans*, when coupled with genetic validation of identified targets to reproduce the small molecule's phenotypic effects, provide a unique platform for discovering the biological targets of compounds that affect multicellular processes. First, the use of an immobilized FK506 derivative and soluble competition experiments with optimally prepared soluble *C. elegans* proteome successfully identified interactions with FK506 binding proteins 1 to 6. This approach was used to determine an unknown mechanism of action for clovanemagnolol, a small molecule that promotes axonal branching in both primary neuronal cultures and *in vivo* in *C. elegans*. Following the synthesis of an appropriately functionalized solid-phase reagent bearing a clovanemagnolol analogue pull-down.

A flow protocol for the generation of phthaloyl peroxide has been developed. This process directly yields phthaloyl peroxide in high purity (>95%) and can be used to bypass the need to isolate and recrystallize phthaloyl peroxide, improving upon earlier batch procedures. The flow protocol for the formation of phthaloyl peroxide can be combined with arene hydroxylation reactions and provides a method for the consumption of peroxide as it is generated to minimize the accumulation of large quantities of peroxide.

JONATHAN J. SILBERG, C-1614, Rice University. REGULATION OF Hsp70 CATALYTIC ACTIVITY BY THE ZINC-FINGER PROTEIN DNLZ/HEP.

Mutations in proteins that synthesize Fe-S clusters can lead to defects in DNA metabolism and genome instability. However, we do not understand how the metallocluster synthesis and degradation change dynamically within living organism's organism or how changes in the sequences and activities of the proteins that regulate iron-sulfur cluster biogenesis impact *in situ* biosynthesis reactions. To better understand these biosynthesis reactions within living cells, we have been investigating whether the fluorescence emission of the near-infrared fluorescent protein (IFP) can be coupled to a protein-protein interaction that is dependent upon coordination of a 2Fe2S cluster. Three libraries of two-piece IFP were generated and screened for variants that display near-infrared fluorescence upon expression within *Escherichia coli*. Screening identified thirteen bipartite IFP that fluoresced, all of which arose from backbone fission proximal to the linker that connects the PAS (Per/ARNT/Sim) and GAF (cGMP phosphodiesterase/adenyl/cyclase/FhIA). All of the bipartite IFP displayed complementation that could be enhanced by fusion to proteins that associate, including IAAL-E3 and IAAL-K3 peptides or CheA and CheY proteins, and the higher affinity IAAL-E3 and IAAL-K3 interaction consistently yielded higher near-infrared fluorescence. These results provide fundamental insight into the locations where IFP can tolerate backbone fission and fusion to proteins that associate. In addition, the bipartite IFP discovered from the measurements can now be used to probe protein-protein interactions that depend on 2Fe2S binding, such as glutaredoxin dimerization *in situ*.

ALEXEI V. SOKOLOV, A-1547, Texas A&M University. APPLICATIONS OF MOLECULAR COHERENCE IN ULTRAFAST OPTICS.

We generate coherent Raman sidebands by crossing two femtosecond laser pulses in a Raman-active crystal. In one experiment, where we use highly-chirped time-delayed input pulses, each sideband is broad enough to produce a spectral overlap with neighboring sidebands, and to form a combined octave-spanning coherent supercontinuum. We control spectral phases of Raman sidebands in a precise and stable manner, so as to allow single-optical-cycle

pulse synthesis and sub-cycle field shaping, to be applied to photoionization and to the area of ultrafast light-matter interactions in general. In addition, we explore spatial beam shaping and generation of optical vortices, opening a possibility for spatio-temporal engineering of sub-cycle pulses. In a separate experiment, we study molecular-frame photoelectron angular distributions from N₂, O₂, and benzene, and illustrate how the angle-dependent ionization rate affects the photoelectron cutoff energy. Our experimental results are supported by an analysis emphasizing the nodal structure of the molecular orbitals.

DONG HEE SON, A-1639, Texas A&M University. DARK EXCITON IN THE ENERGY TRANSFER PROCESS OF SEMICONDUCTOR NANOCRYSTALS.

In this project year, our investigation focused on two subjects: (i) Recovery of the trapped exciton as photon via energy transfer from trapped exciton to dopant in doped semiconductor nanocrystals, (ii) photoinduced separation of the strongly interacting layered transition metal dichalcogenide nanocrystals. For the first topic, we found out that the trapped excitons in semiconductor quantum dots that are usually wasted as heat after the photoexcitation, limiting the quantum yield, can be recovered as photon by using thiol surface ligand as the facilitator that enables the sensitization of the trapped exciton to dopant. This is unexpected since thiol ligands usually reduce the quantum yield of the undoped nanocrystals by trapping the exciton. However, thiols in doped quantum dots play dual roles, i.e., hole trap and facilitator of the sensitization of trapped exciton, resulting in the net enhancement of quantum yield in doped quantum dots. The ligand-assisted recovery of the trapped exciton as the sensitized photon is particularly beneficial when utilizing the doped quantum dots as the light emitting element. For the second topic, we discovered that the strong interparticle interaction in colloidal 2-D transition metal dichalcogenide (TMDC) nanodiscs that forms the assembly of the interacting particles can be controlled via photoexcitation. The assembly of the interacting particles that interferes with the characterization of the individual non-interacting 2-D TMDC nanodiscs can be resolved by modifying the cohesive force between the particles via photoexcitation. We found out that dense charge carriers from the photoexcitation weaken the interparticle cohesive force facilitating the solvation of each particle by the solvent molecules.

ZHOU SONGYANG, Q-1673, Baylor College of Medicine. NOVEL ACTIVITY OF THE TELOMERE REGULATOR TIN2 IN THE MITOCHONDRIA.

At the ends of eukaryotic chromosomes are specialized structures called telomeres, which are important for maintaining genome stability and integrity. Extensive studies have been carried out to illustrate how core telomeric proteins assemble on telomeres to recruit the telomerase and additional factors for telomere maintenance and protection in mammalian cells. In comparison, how changes in growth signaling pathways impact telomeres and telomere-binding proteins remains largely unexplored. The phosphatidylinositol 3-kinase (PI3-K)/Akt (also known as PKB) pathway, one of the best characterized growth signaling cascades, regulates a variety of cellular function including cell proliferation, survival, metabolism, and DNA repair, and dysregulation of PI3-K/Akt signaling has been linked to aging and diseases such as cancer and diabetes. During the last grant period, we provide evidence that the Akt signaling pathway plays an important role in telomere protection. Specifically, Akt inhibition either by small molecule inhibitors or small interfering RNAs induced telomere DNA damage and disrupted telomere length regulation. Furthermore, we found that TPP1 could homodimerize through its OB fold, a process that was dependent on the Akt kinase. Telomere damage and reduced TPP1 dimerization as a result of Akt inhibition was also accompanied by diminished recruitment of TPP1 and POT1 to the telomeres. Our findings highlight a previously unknown link between Akt signaling and telomere protection, and point to novel mechanisms for regulating TPP1-mediated telomere control. This work was published on *Aging Cell*.

The mature and active telomerase complex is assembled in Cajal bodies, which are specialized and dynamic compartments in the nucleus that are involved in the biogenesis of small nuclear ribonucleoproteins (snRNPs). We reasoned that proteins localized to Cajal bodies could participate in telomerase biogenesis. In collaboration with Dr. Junjie Chen at MD Anderson Cancer Center, we carried out a genome-wide screen to identify proteins that co-localize with coilin, the marker protein of Cajal bodies. This work was published on *JCB*. One of the novel Cajal body proteins discovered is Fam118B. Fam118B is widely expressed in a variety of cell lines derived from various origins. Overexpression of Fam118B changes the canonical morphology of Cajal bodies, whereas depletion of Fam118B disrupts the localization of components of Cajal bodies, including coilin, the survival of motor neuron protein (SMN) and the Sm protein D1 (SmD1, also known as SNRPD1). Moreover, depletion of Fam118B reduces splicing capacity and inhibits cell proliferation. In addition, Fam118B associates with coilin and SMN proteins. Fam118B depletion reduces symmetric dimethylarginine modification of SmD1, which in turn diminishes the binding of SMN to this Sm protein. Taken together, these data indicate that Fam118B, by regulating SmD1 symmetric dimethylarginine modification, plays an important role in Cajal body formation, snRNP biogenesis and cell viability. This work was published on *JCS*.

JOHN F. STANTON, F-1283, The University of Texas at Austin. STUDIES IN QUANTUM CHEMISTRY.

Our Welch-supported research during the 2013-2014 funding period has been quite productive, and has involved work in areas ranging from fundamental algorithm development for spectroscopic simulations to quantum-chemical method development to collaborations with experimentalists where our theoretical tools have been used to understand and interpret various types of molecular spectroscopy. The latter works have largely dealt with organic molecules; the two highlights of the previous year were to study the so-called Criegee molecule (CH₂COO) with the McCarthy group at Harvard University and hydroxycarbene (HCOH) with the Doublerly group at the University of Georgia. Both of these molecules have only been discovered recently and both have assumed important roles in the atmosphere. In other work, we have continued our longstanding studies of vibronic coupling in molecules, working on the interesting cation of para-benzoquinone (OC₆H₄O⁺) with T. Bally in Switzerland and the methoxy radical with the Neumark group at Berkeley.

We have also implemented massive parallelization of vibronic coupling calculations, which was presented as a poster at the Sanibel Symposium for Quantum Chemistry in the Spring of 2014. This work has led to a code that can – given a large-scale computational resource like those available at TACC in

Austin – apply the Lanczos diagonalization procedure to a matrix with dimensions of order 10^6 and promises to open up exciting new capabilities in our work on molecular spectra.

We are also continuing to work on the high-level coupled-cluster methods based on the CCSDTQ approximations. The energy code is finished (with a paper in submission) and we are working now on analytical gradient methods.

MIHAELA C. STEFAN, AT-1740, The University of Texas at Dallas. POLYTHIOPHENE BLOCK COPOLYMERS: A SYSTEMATIC INVESTIGATION OF MORPHOLOGY – OPTOELECTRONIC PROPERTIES DEPENDENCE.

During the fourth year of my proposal we have synthesized polyisoprene-*b*-polystyrene-*b*-poly(3-hexylthiophene) (PI-PS-P3HT) triblock copolymer by anionic coupling of *living* polyisoprene-*b*-polystyryl lithium with allyl-terminated poly(3-hexylthiophene). The triblock copolymer preserved the opto-electronic properties and morphology of poly(3-hexylthiophene) homopolymer despite the presence of the insulating polyisoprene and polystyrene blocks. Nanofibrillar morphology was observed for the PI-PS-P3HT thin film deposited from toluene. A field-effect mobility of $5.0 \times 10^{-4} \text{ cm}^2/\text{Vs}$ was measured for the untreated OFET device. We collaborated with Dr. Zhiqun Lin from Georgia Institute of Technology to investigate the self-assembly of this triblock copolymer at the air-water interface by Langmuir-Blodgett (LB) technique. The obtained monolayer thick film exhibited high photoluminescence which was attributed to the successful transferring of the amorphous P3HT side chains in the PI-PS-P3HT triblock copolymer from the solution to solid state. We found that the increase in the lateral surface pressure resulted in the chaining of the aggregates which was attributed to the competition between the short range attractive forces of hydrophobic PI and PS aggregates and the long range repulsive forces generated by the spread of the P3HT monolayer. This LB promoted self-assembly of polythiophene block copolymers is currently investigated in my group and it is expected to generate a versatile method to fabricate thin film devices with improved optoelectronic properties. We have published a paper in collaboration with Dr. Zhiqun Lin to report this research and we are currently testing other P3HT block copolymers for LB self-assembly.

KEITH J. STEVENSON, F-1529, The University of Texas at Austin. SYNTHESIS OF MESOPOROUS CARBON AND METAL OXIDE ARCHITECTURES.

Over this grant period we have continued to explore new approaches for preparing nanostructured, mesoporous carbons, metal oxides and transition metal phosphates such as LaMnO_3 , and $\text{Li}_3\text{V}_2(\text{PO}_4)_3$. New oxide and phosphate materials with unique valence states have been prepared by hydrothermal synthesis; while nanostructured LaMnO_3 and LaCoO_3 have been prepared using reverse phase precipitation in collaboration with Prof. Keith P. Johnston. Both methods allowed us to tune micro- and nano-crystalline phase domains within the metal oxides to exert influence over materials properties including, optical, ionic and electrical conductivity. The oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) mechanisms at nitrogen doped nanocarbons supports have been investigated in several studies. A complex surface-mediated ORR mechanism involving a dual site reduction has been elucidated for nitrogen doped carbons. Nitrogen doped nanocarbons have also allowed for highly quantitative detection of glucose, FAD, and NADH due to their unique catalytic activity. Finally, we have also developed several new electrodeposition methods for depositing thin film metal chalcogenides (MoS_2 , MoSe_2 , and Se).

PAUL D. STRAIGHT, A-1796, Texas A&M University. IDENTIFICATION OF ANTIBIOTIC RESISTANCE AND MODIFYING ENZYMES FROM BACTERIAL COMPETITIVE INTERACTIONS.

Over the past year we have focused on (Objective 1) the surfactin hydrolase enzyme (SfhA), which we identified and described in Hoefler et al., 2012, *PNAS*, and on (Objective 2) developing experimental conditions and formats for identifying antibiotic resistance mechanisms. In the case of SfhA, we recognized during the course of genome sequencing *Streptomyces* sp. Mg1 (Hoefler et al, 2013, *Genome Announcements*), the SfhA producer, that the mature protein has an extended N-terminus responsible for secretion and processing. This finding is significant because it suggests that active protein is obtainable without *in vitro* denaturation and refolding, as we described previously. We reconstructed expression systems in both *Streptomyces* sp. Mg1 and *E. coli*. The *E. coli* system produces abundant SfhA protein, including a soluble active fraction required to characterize of this enzyme using both surfactin and daptomycin as substrate molecules. Our preliminary data suggests that the enzyme substrate selectivity is dependent upon environmental conditions. This finding has significant implications for our understanding of the evolution and adaptation of enzymatic mechanisms of antibiotic resistance. In the case of Objective 2, we have analyzed multiple interactions between *Bacillus* sp. and *Streptomyces* sp. under differing conditions of culture and incubation to determine formats for screening by imaging mass spectrometry and identify pairs for developing screens. We have identified conditions where morphological changes (motility, biofilm formation, spore development) are visible, and raise the probability of detecting mass shifts associated with enzyme functions.

WU-PEI SU, E-1070, University of Houston. A REAL SPACE APPROACH TO THE MACROMOLECULAR PHASE PROBLEM.

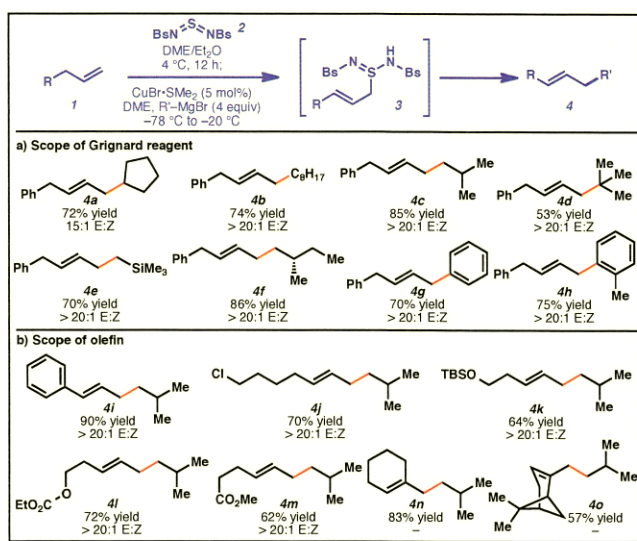
We have discovered a new method for solving the phase problem in protein crystallography. A very powerful algorithm for retrieving the phases, the so-called hybrid input-output (HIO) method, has been widely applied in optical imaging and X-ray diffraction imaging of small samples. The algorithm can determine the phase from the magnitude of a diffracted wave because the sample is localized in a small region in space. In a protein crystal, the region between the proteins is usually occupied by the solvent which has a constant electron density. It turns out that also imposes a strong constraint on the phase of a diffracted wave. We have adapted the HIO method to take advantage of this constraint. Our trial calculations have shown that the method can successfully retrieve the phases and therefore is capable of generating high resolution images of proteins from the diffraction pattern alone, provided that the protein crystal has a high solvent content. More precisely, that means the solvent occupies at least half of the total volume of the crystal. Although the result needs to be consolidated and extended to have a wider applicability, it is a very important result and it suggests that we may be close to solving a long-standing problem in

X-ray crystallography.

One way to overcome the solvent content restriction is to utilize the non-crystallographic symmetry (NCS) that is frequently present in a protein crystal. Our preliminary result shows that is feasible. We have also attempted to combine the previously developed real space approach with the HIO phasing algorithm to eliminate major restrictions of the current methodology.

UTTAM K. TAMBAR, I-1748, The University of Texas Southwestern Medical Center. STEREOSELECTIVE ALLYLIC FUNCTIONALIZATION OF OLEFINS.

The functionalization of unactivated olefins with carbon nucleophiles has emerged as an attractive alternative to traditional Heck reactions for the conversion of terminal olefins into more complex internal olefin products with functional groups. Based on our initial proposal, we have explored a novel strategy for the allylic functionalization of unactivated olefins, which is based on our previous work supported by the Welch Foundation (Grant 1-1748). We have employed copper catalysts in the selective allylic alkylation of unactivated olefins with Grignard reagents to generate internal olefins with high *E*-selectivity (see Figure). The transformation is compatible with several functional groups, including alkylsilanes, chlorides, silyl ethers, carbonates, and esters. This represents a general method for functionalizing unactivated olefins with aromatic, aliphatic, and vinyl Grignard reagents. We have synthesized a series of skipped dienes, a class of compounds that are present in many natural products and are difficult to synthesize by known allylic alkylation methods.



YIZHI JANE TAO, C-1565, Rice University. CATALYTIC MECHANISM OF ASTROVIRUS RNA REPLICATION.

We have now completed our biochemical characterization of the astrovirus VPg nucleotidyl transferase activity. Mutation of a potential nucleotide acceptor motif ²⁵LTEEEYRE identified residue E29 essential for VPg nucleotidyl transferase activity. Mutation of E27 and E28 also significantly reduced the VPg activity. We found that the first 20 and the last 28 residues of VPg were dispensable for VPg nucleotidyl transferase activity. VPg could react with not just UTP, but also GTP and CTP. Our study of the astrovirus protein priming thus revealed several distinct mechanistic features compared to picornaviruses. X-ray structure determination of the astrovirus polymerase and VPg are in progress.

Meanwhile, we have made excellent progress in our study of the RNA-dependent RNA polymerase (RdRP) from a small double-stranded (ds) RNA virus, the picobirnavirus, which infects a wide range of mammalian and avian species and has been associated with acute gastroenteritis in children and immunocompromised patients. During the replication cycle dsRNA viruses, the viral RdRPs replicate and transcribe the viral genome from within the confines of a viral capsid. In this study, we have determined a 2.4 Å resolution structure of an RdRP from the human picobirnavirus (hPBV). In addition to the conserved polymerase fold, the hPBV RdRP possesses a unique, highly flexible 24 amino acid loop structure located near the C-terminus of the protein that is inserted into its active site. Through *in vitro* RNA polymerization assays and site-directed mutagenesis, we have shown that the insertion loop likely functions as an assembly platform for the priming nucleotide to facilitate *de novo* RNA synthesis. We are currently working on the crystal structure of several hPBV RdRP catalytic complexes to determine how the insertion loop changes its conformation during the initiation and elongation stages of the viral RNA replication process. We expect that our studies of the hPBV will help to define a new paradigm for the assembly and replication of small dsRNA viruses in which the viral RdRP most likely functions independently of the viral capsid.

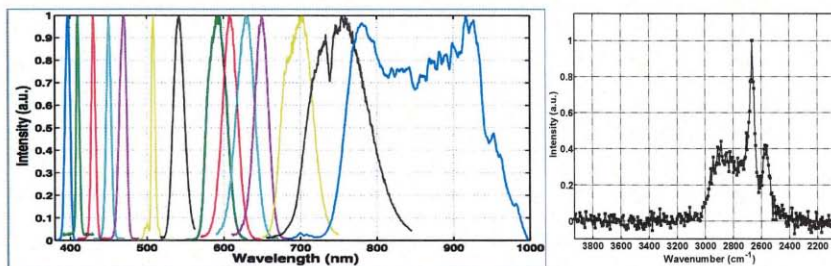
JONATHAN R. TERMAN, I-1749, The University of Texas Southwestern Medical Center. CHEMISTRY AND ENZYMOLOGY OF MICAL FAMILY OXIDOREDUCTASES.

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 alter 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 this oxidation-reduction (Redox) reactions are poorly defined. Interestingly, in our attempt to characterize the biochemical signals that alter cellular motility, we have identified a novel family of proteins, the MICALs, whose members are similar at the amino acid level to Redox enzymes. We have previously found that MICALs are critical for the shape, motility, and guidance of cells - and provide a long-sought direct physical and functional link between one of the largest families of extracellular guidance cues (the semaphorins and their Plexin cell surface receptors) and the modification of the cell's internal skeleton (the actin cytoskeleton). Our work with the support of the Welch Foundation has gone on to reveal (as *described by others*) a "...completely new mechanism by which actin dynamics can be altered" and "...adds to the list of posttranslational modifications that effect the regulation of cellular behavior". Now, over the past year, we find that this new mechanism is reversible - and this is accomplished by a family of enzymes called MsrBs (also called SelRs). Specifically, our work reveals that Mical oxidizes actin stereo-specifically to generate actin Met-44-R-sulfoxide (actin^{Met(R)O-44}) and MsrB/SelR reverses these effects both *in vitro* and *in vivo*. Our work is thus the first to discover that the interconversion of specific Met/Met(R)O residues is a precise means to control protein function and uncovers a novel and specific reversible Redox actin regulatory system. These results reveal a new reversible post-translational mechanism controlling biology.

ISABELL THOMANN, C-1825, Rice University. ANVANCED FEMTOSECOND OPTICAL *IN SITU* PROBES FOR PHOTOCATALYSIS.

In summer 2013, my graduate student Chloe Doiron travelled to Munich, Germany to help construct a worldwide-unique laser system (noncollinearly pumped optical parametric amplifier, NOPA). The finalized NOFA was installed at Rice University in February 2014, and supports sub-15 fs pulses with wavelength tuning range from 395 nm to 1000 nm (see left figure panel). Based on this laser system, we have constructed a FSRS setup that can probe Raman active molecular vibrations between 300 and 3000 cm^{-1} . To characterize the setup, we have acquired stimulated Raman spectra of methanol with a picosecond Raman probe pulse and a broadband femtosecond Raman pump pulse. The signal was detected using a noncollinear geometry with an interaction length of only ~500 microns. Careful instrument calibrations are currently being pursued. After lab renovations were completed in September 2013, we began to install equipment and synthesized photoanode and photocathode materials for solar water splitting employing plasmonic nanostructures and two-dimensional materials. These structures were carefully designed for extreme light absorption at the electrode/aqueous solution interface and will be characterized by the FSRS setup.

Figure 1: left: NOPA laser spectra; right: stimulated Raman signal from methanol;



RANDOLPH P. THUMMEL, E-0621, University of Houston. THE DESIGN AND SYNTHESIS OF AZAAROMATIC LIGANDS AND THE STUDY OF THEIR METAL COMPLEXES.

We have continued our investigation into the mechanism and performance of a wide range of mono-nuclear Ru(II) complexes as light-driven water oxidation catalysts. In probing the intermediacy of a seven coordinate Ru(IV) species, we have noted the important role of steric effects. Tridentate ligands that impede the formation of pentagonal bipyramid geometry also inhibit water oxidation. In this regard a new class of tridentate 6,5-chelators are being carefully investigated.

We have prepared a series of molecular dyads in which an oxidation catalyst and a photosensitizer are connected through an appropriate bridging ligand. Light-driven water oxidation is observed when the excited state reduction potential of the sensitizer is greater than the first oxidation potential of the catalyst.

An approximately planar tetradentate polypyridine ligand, 8-(1",10"-phenanthroline-2"-yl)-2-(pyridin-2'-yl)quinoline (ppq), has been prepared by two sequential Friedländer condensations. The complex [Co(ppq)Cl₂] in pH 4 aqueous solution, together with the photosensitizer [Ru(bpy)₃]Cl₂ and ascorbic acid as a sacrificial electron donor, in the presence of blue LED light ($\lambda_{\text{max}} = 469 \text{ nm}$) produces hydrogen with a initial TOE = 586 h^{-1} .

Together with Sherri McFarland at Acadia University, several mononuclear Ru(II) dyads possessing 1,10-phenanthroline-appended pyrenyl ethynylene ligands were synthesized, characterized, and evaluated for their potential in photodynamic therapy. We continue our fruitful collaborations with the group of Etsuko Fujita at Brookhaven National Laboratory and Jacek Waluk at the Polish Academy of Sciences.

CHIN-SEN TING, E-1146, University of Houston. STUDY OF SUPERCONDUCTIVITY AND RELATED SUBJECTS IN STRONGLY CORRELATED ELECTRON SYSTEMS.

Considering the coexistence of the 2×1 colinear spin-density-wave (SDW) and superconductivity (SC) with the S_{\pm} pairing symmetry in iron-pnictide superconductors like $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$, $\text{CaFe}_{2-x}\text{Co}_x\text{As}_2$ and $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, we developed an improved two orbital-model which breaks the symmetry of the tetragonal point group by lowering it from C_4 to D_{2d} for the purpose to compare with the angular resolved photoemission experiments. It properly describes the electronic structures of both electron and hole doped compounds. Based on this model we performed a comprehensive investigation of the evolution of the Fermi surface (FS) topology in the presence of the SDW order as the doping is changed. In the parent compound ($x=0$), the ground state is the SDW order, where the ES is not completely gapped, and two types of Dirac cones, one electron-doped and the other hole-doped, emerge in the magnetic Brillouin zone. Our findings are qualitatively consistent with recent angle-resolved photoemission spectroscopy and magneto-resistivity measurements. The ES evolutions of both electron- and hole-doped samples are investigated and the obtained theoretical results are compared successfully with measurements. The effect of Zn-impurities, which replace Fe atoms in the compound, has also been studied. We demonstrate that the SC is completely suppressed in the doped BaFe_2As_2 compounds with an approximately 10% Zn impurity concentration. This result is in agreement with experiments and also indicates the SC in these compounds may be of S_{\pm} pairing symmetry. In addition we also studied several related problems like the topological phase transition in certain compounds, the possible spin-polarized-current state in bilayer graphene, and the interaction-induced localization of mobile impurities in ultra cold atom systems.

FRANK K. TITTEL, C-0586, Rice University. APPLICATION OF MID-INFRARED QUANTUM CASCADE AND DIODE LASERS TO HIGH-PRECISION ATMOSPHERIC TRACE GAS MONITORING.

Several projects from the previous year were completed and resulted in publications. A $7.83 \mu\text{m}$, continuous wave, distributed feedback, high power ($>120\text{mW}$) QCL QEPAS sensor platform employing 2f detection for ultra-sensitive detection of CH_4 and N_2O was developed. For the targeted CH_4 and N_2O absorption lines located at 1275.04 cm^{-1} and 1275.49 cm^{-1} the minimum detectable concentration (MDC) was determined to be 13 ppbv and 6 ppbv, respectively for a 1 s. data acquisition time. This sensor was installed in a mobile laboratory operated by Aerodyne Research, Inc to perform atmospheric CH_4 and N_2O concentration measurements near two Greater Houston area landfills during the 2013 NASA field campaign *DISCOVER-AQ*. Compared to typical ambient atmospheric mixing ratios of CH_4 and N_2O of 1.8 ppmv and 321 ppb, respectively, increases in mixing ratios of ~ 53 ppmv for CH_4 and an increase of ~ 350 ppbv for N_2O were observed when the mobile laboratory circled two waste disposal sites located in Harris County, TX. Furthermore a QEPAS sensor was developed for the detection of H_2O_2 , identified as an important atmospheric species playing a major role in the oxidative capacity of the atmosphere and the balance of HO_x radicals at an absorption line located at $\sim 7.73 \mu\text{m}$. Sensor calibration was performed using a water bubbler that generated titrated average H_2O_2 vapor concentrations. A MDC of 75 ppbv with a 1 s integration time was achieved.

ZACHARY J. TONZETICH, AX-1772, The University of Texas at San Antonio. COORDINATION CHEMISTRY OF HYDROGEN SULFIDE RELEVANT TO BIOLOGY.

Our work over the last year (grant year 3) has continued to examine in detail the interactions of hydrogen sulfide and its derivatives with synthetic transition metal complexes. We have exciting unpublished data concerning the first example of an iron(II) porphyrinate- H_2S complex, which we have crystallographically characterized. Work is continuing to fully characterize this species and determine the binding constant for H_2S . We have also started examining the reactivity of hydrosulfide ion, (HS^-), with iron porphyrinates containing nitric oxide. These studies will elucidate the reaction pathways available to H_2S when it encounters NO in the presence of metal ions. In addition to our ongoing work, we have also published three papers in the last grant year with the support of the Welch Foundation. In one publication we describe the chemistry of iron(III) porphyrinates containing silanethiolate ligands. Silanethiols are used as electronically similar but sterically more encumbering analogs of H_2S . In a second publication, we report a new PNP pincer ligand platform and its chemistry with Ni(II). We have subsequently used this ligand platform to stabilize a rare example of a nickel hydrosulfide complex, work that is submitted for publication. In our third publication, we describe an improved synthesis of iron(III) porphyrinates containing fluoride ligands. The fluoride compounds were first prepared during the course of our investigations with silanethiols, but we have now developed an improved procedure for their synthesis, which is markedly better than existing methods.

THOMAS M. TRUSKETT, F-1696, The University of Texas at Austin. LIQUIDS NEAR INTERFACES: SINGLE-MOLECULE AND COLLECTIVE DYNAMICS.

We completed research this year that provides insights into the structure and dynamics of molecular liquid and complex fluid systems (e.g., nanoparticle and colloidal suspensions) where interfaces play an important role. In one study, we used molecular simulation to identify and characterize qualitatively different dynamical diffusion processes that occur in confined fluids under conditions corresponding to distinct structural regimes (film formation, multilayer adsorption, and pore-filling). In a second study, we demonstrated how isomorph theory can help predict the implications of supercooling or overcompression on the thermodynamic and transport properties of dense confined fluids. A third investigation showed how targeted self-assembled lattice structures with good thermal stability can be obtained by designing nanoparticle interactions which stabilize the desired structures as ground states over a wide density range. A fourth study established a new and general approach for predicting thermodynamic and structural properties of complex fluids via a strategy that combines integral equation theory with a pair-potential discretization. In a fifth study, we demonstrated how to self-assemble NIR-active, biodegradable nanoclusters of gold primary particles of interest for biomedical imaging with sizes and morphologies that are tunable via solution pH and ionic strength. In a

final study, we showed how various nanoparticle surfactant combinations can be designed to greatly enhance the stability of oil-in-seawater emulsions using very low surfactant loadings.

FRANCIS T.F. TSAI, Q-1530, Baylor College of Medicine. STRUCTURAL AND MECHANISTIC STUDIES OF ATP-DRIVEN PROTEIN MACHINES.

Multi-subunit, ATP-dependent molecular machines are difficult to study because of their large size and inherent conformational plasticity. Current targets include ATP-dependent molecular chaperones, energy-dependent proteases, and nuclease-helicases. A major limitation in crystallographic work is the need to capture or trap these machines in a distinct conformation that is amenable for structural analysis. To develop new chemical probes against molecular chaperones, we have screened a library of small molecule compounds against Hsp90 at the John S. Dunn Gulf Coast Consortium for Chemical Genomics. The most promising compounds belong to a family of plant-derived flavonoids that bound Hsp90 with nanomolar affinity (~500 nM) and induced cell death of LNCaP prostate cancer cells with an IC_{50} in the micromolar range (~80 μ M). Structure-activity relationship studies by *in silico* ligand docking confirmed that our identified flavonoids compete with ATP for binding to Hsp90, and suggested new avenues how to improve the specificity of these compounds by adding new functional groups. In parallel, crystallization trials have yielded small crystals of one inhibitor complex, which diffracted to 3.15-Å resolution using our in-house X-ray source. We are currently optimizing our initial crystal hit in order to collect a complete, high-resolution data set at the national synchrotron-radiation light source in Argonne, IL.

BENJAMIN P. TU, I-1797, The University of Texas Southwestern Medical Center. SELECTIVE REGULATION OF AUTOPHAGY BY METABOLIC STATE.

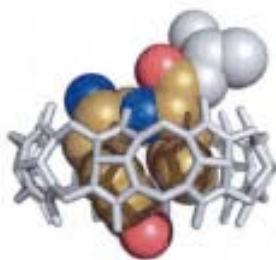
Using prototrophic strains of yeast, we discovered when cells are switched from a rich to minimal culture media that is still fully capable of supporting growth, they induce autophagy as a means of cellular homeostasis. We termed this form of autophagy, non-nitrogen-starvation autophagy (NNS-autophagy), since it occurs in the absence of typical nitrogen starvation conditions, in response to more subtle changes in the nutrient environment. Using a visual screen, we discovered NNS-autophagy is specifically regulated by a conserved complex of three proteins, Iml1p, Npr2p, and Npr3p. The human ortholog of Npr2p lies in a genomic region that is frequently deleted in cancers, and has been described as a tumor suppressor. Notably, yeast *npr2* Δ mutants exhibit dysregulated growth reminiscent of cancer and recent studies place the Npr2-containing complex as an upstream negative regulator of TORC1. In efforts to understand the nutritional trigger of NNS-autophagy, we observed that a single amino acid, methionine, is sufficient to block this process. No other amino acid, including glutamine or leucine, is active in this regard. We traced the effects of methionine specifically to a downstream metabolite, S-adenosylmethionine (SAM). We then deduced that methionine and SAM inhibit autophagy through the action of a conserved methyltransferase that modifies the catalytic subunit of Protein Phosphatase 2A (PP2A). We now understand that this modification is driven by SAM levels and enables the subsequent regulation of protein phosphorylation (one substrate of methylated PP2A is Npr2p) in tune with methionine/SAM availability. Collectively, our findings show that these sulfur-containing metabolites constitute a previously unrecognized gauge of cellular metabolic state and amino acid sufficiency. This discovery has significant implications for our understanding of the regulation of cell growth and lifespan by amino acids.

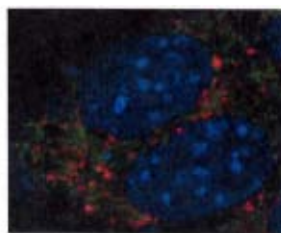
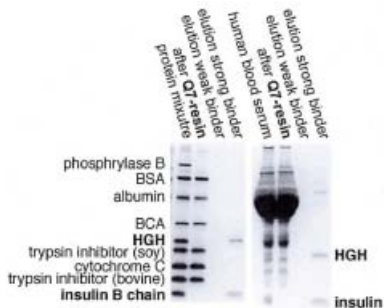
ADAM R. URBACH, W-1640, Trinity University. PROTEIN RECOGNITION AND LABELING VIA SUPRAMOLECULAR PROTEASE INHIBITION.

Substantial progress was made on several proposed goals. We showed that the cucurbit[7]uril-loaded resin described in the proposal can isolate the phenylalanine-terminated proteins insulin and human growth hormone (HGH) selectively from simple protein mixtures and from enriched blood serum.

A novel combinatorial screen yielded a peptide sequence (Tyr-Leu-Ala) that binds cucurbit[8]uril with a dissociation constant of 7 nM and at least 5000-fold sequence-specificity, which is, to our knowledge, the highest peptide affinity and sequence specificity reported for a synthetic receptor. Structural studies revealed a novel binding motif in which neighboring Tyr and Leu residues fold tightly, bind in the cavity, and stabilize the complex with five hydrogen bonds.

We synthesized the first cucurbituril-dye conjugates and showed that they can sense analytes in the low nanomolar range without paying the energetic penalty for dye dissociation. We added the conjugates to live HT22 neurons and saw uptake and localization to mitochondria.





KOSAKU UYEDA, I-1720, The University of Texas Southwestern Medical Center. **BIOCHEMICAL MECHANISM OF THE GLUCOSE SENSING AND REGULATION OF ChREBP ACTIVITY.**

ChREBP-dependent gene transcription is controlled by ChREBP trafficking between cytosol and nucleus and by altered efficiency of ChREBP binding to carbohydrate responsive elements in targeted genes. The nuclear/cytosol shuttling is carried out by N terminal region (amino acids 1-250) of ChREBP and the same region is responsible for glucose sensing. We showed that the nuclear export process under low glucose involves phospho-ChREBP complex with 14-3-3, then the heterodimer binds to CRM1, while nuclear import involves dephospho-ChREBP forms a complex with importin alpha then the complex binds to importin beta. 14-3-3 has two binding sites on ChREBP, primary and secondary, and appears to be bound to the primary site of ChREBP regardless of glucose concentration while the secondary binding site for 14-3-3 competes with importin alpha and when phosphorylated on Ser196 it inhibits importin binding, and regulates nuclear/cytosol trafficking by sensing the changes in glucose levels. We have found a metabolite which enhances binding of 14-3-3 to ChREBP, and the metabolite was identified as ketone body and amplifies inhibition of nuclear import during the starvation to insure that ChREBP is inactive and remains in the cytosol. We will continue to investigate the Biochemical mechanism of the glucose sensing.

AMBRO VAN HOOFF, AU-1773, The University of Texas Health Science Center at Houston. **EXOSOME ACTIVATION BY THE ATPASE AND POLY(A) POLYMERASE ACTIVITY OF THE TRAMP COMPLEX.**

We proposed to characterize how these two subunits interact to form the TRAMP complex, disrupt the interaction and finally characterize the functional consequences of this interaction. We have completed large parts of this project. Specifically, using *in vivo* and *in vitro* approaches we have shown twenty amino acid peptides of poly(a) polymerase is required and sufficient for interaction with ATPase both *in vitro* and *in vivo*. Furthermore, we have shown that disrupting this interaction has no effect on growth and only modest effects on TRAMP function. During the last year we have studied the effect of disrupting this interaction on specific RNA processing and degradation events, by Northern blotting and qrt-PCR. Some of these findings need to be confirmed. We are also planning to use transcriptome sequencing as a more unbiased approach during the no-cost extension period.

NAVIN VARADARAJAN, E-1774, University of Houston. **ENGINEERING CHYMOTRYPSIN TO SELECTIVELY CLEAVE AFTER PHOSPHOTYROSINE.**

Engineering of chymotrypsin to recognize pTyr. We focused on re-engineering the substrate specificity of rChyB to selectively recognize pTyr, not only to enable the creation of catalysts that could be used as proteomic tools but also to facilitate a basic understating of the rules of molecular recognition. A site-saturation library simultaneously targeting four residues that comprise the bottom of the Si substrate binding pocket, was constructed and *E. coli* MC1061 cells expressing ChyB variants displayed on the surface were isolated using two-color selection/counter-selection flow-cytometry, utilizing FRET substrates that harbor a protease sensitive site. Subsequent to six rounds of sorting, single colonies were obtained and DNA sequencing of ChyB-phos variant demonstrated the presence of two positively charged Arg residues within the modified substrate binding pocket, presumably facilitating recognition of pTyr through ion-pair interactions. HPLC characterization however did not indicate that the variant was catalytically active and we are currently employing other libraries to try and screen for more active variants.

Engineering of chymotrypsin to recognize Asn. We attempted in parallel, to engineer the substrate specificity of Asn and isolate ChyB-Asn that can be used as a tool for mapping of glycosylation sites. Based on the crystal structure of chymotrypsin in complex with a substrate analogue, eleven residues in the extended substrate binding pocket were identified for randomization while carefully avoiding residues considered critical for catalytic activity as they were conserved across proteases with chymotrypsin fold but differing substrate specificities. *E. coli* MC1061 cells expressing ChyB variants were screened as previously to isolate ChyB-Asn with 9 amino acid substitutions. Fragments of FRET substrate generated by proteolysis were analyzed LC-MS to verify the specificity of ChyB-Asn. To improve kinetics by reverting deleterious or neutral mutations, we screened a library obtained by backcrossing ChyB-Asn with wild-type ChyB to isolate ChyB-Asn 1.1 which displayed 2.5 fold higher activities than ChyB-Asn. These results, albeit without kinetic parameters, suggest that modulating substrate specificity of ChyB towards variety of novel substrates should be feasible.

YIHONG WAN, I-1751, The University of Texas Southwestern Medical Center. BIOCHEMICAL CHARACTERIZATION OF PAFAH REGULATION BY MACROPHAGE VLDLR.

During the first year of our studies supported by the Welch Foundation, my laboratory has further investigated the cellular and biochemical mechanism for how maternal VLDLR regulates milk PAFAH levels and prevents neonatal inflammation. First, we have elucidated that VLDLR regulation of PAFAH expression in macrophages was mediated by reelin ligand and Dab2 signaling pathway. These findings reveal novel factors that contribute to VLDLR regulation of macrophage function and milk immunity. Second, we have found that the neonatal inflammation and alopecia triggered by maternal VLDLR deficiency can be rescued by toll-like-receptor 4 (TLR4) deletion or an mTOR signaling inhibitor rapamycin. These findings establish preclinical evidence that inhibitors for TLR4 or mTOR may represent novel therapeutic strategies for the treatment of related infantile disorders. Third, our investigations of VLDLR- and PPAR γ -deficient mice have inspired us to identify additional factors, both maternal and neonatal, that serve as key regulators of the milk-neonate axis to prevent neonatal inflammation. Using neonatal alopecia as visual readout, we have identified maternal factors such as the adipokine adiponectin as an important regulator of milk quality, as well as offspring factors such as the critical mitochondrial complex I subunit NADH: ubiquinone oxidoreductase iron-sulfur protein 4 (Ndufs4) as an important regulator of the postnatal metabolic adaptation to the normal milk from WT mothers. By combining *in vivo* mouse genetic and pharmacological models, *in vitro* cell-based assays, and biochemical analyses such as metabolomics profiling, our future investigations supported by the Welch foundation will further enhance our understanding of the metabolic control of lactation and biochemical regulation of inflammation.

JIN WANG, Q-1798, Baylor College of Medicine. PLASMON ASSISTED PHOTONANOMEDICINES FOR CANCER THERAPIES.

The ultimate goal is to advance current drug delivery technology and improve cancer therapies. With the Welch support, we are developing new drug delivery strategies based on new chemistry and plasmon effect.

Advancement of RNAi therapies is mainly hindered by the development of efficient delivery vehicles. The ability to create small size (<30 nm) oligonucleotide nanoparticles is essential for many aspects of the delivery process but is often overlooked. We developed diblock star polymers that can reproducibly complex double stranded oligonucleotides into monodisperse nanoparticles with 15, 23, or 30 nm in diameter. The polymer-nucleic acid nanoparticles have a core-shell architecture with dense PEG brush coating. We characterized these nanoparticles using ITC, DLS, FRET, FCS, TIRF, and TEM. In addition to small size, these nanoparticles have neutral zeta-potentials, making the presented polymer architecture a very attractive platform for investigation of yet poorly studied polyplex size range for siRNA and antisense oligonucleotide delivery applications. This part of work has been published in *J. Am. Chem. Soc.*, 2014, 136, 234-240. We are currently exploring the *in vivo* behavior of these sub-30 nm nanoparticles. Gold nanoparticles can be combined with these siRNA nanoparticles to enhance delivery efficacy.

Following our previous work on thioesters based "reductive" responsive chemistry for drug delivery (*J. Am. Chem. Soc.*, 2013, 135, 10938-10941), we also developed a series of retro-Michael addition based chemistry for controlled drug release. This chemistry can also be used for reversible protein PEGylation and crosslinking of nanoparticles. This retro-Michael addition based chemistry is highly tunable. We have extensively studied this reaction using physical organic methodology. This part of work is being prepared for submission.

QINGHUA WANG, Q-1829, Baylor College of Medicine. CHEMICAL MECHANISMS OF COORDINATED EPIGENETIC REGULATIONS IN CELLS.

PcG and TrxG are master epigenetic regulators that catalyze trimethylation of histone 3 lysine 27 and lysine 4, respectively, to mark the corresponding genes for transcriptional repression or activation. Without DNA-binding proteins within them, these large protein complexes are believed to utilize DNA-binding transcription factors for their recruitment to thousands of target genes in mammalian genomes. However, the mechanisms by which DNA-binding transcription factors coordinate the binding of PcG and TrxG remained very poorly understood. Therefore, structural and functional studies of ZH, a novel DNA-binding transcription factor newly discovered and characterized in our group, with its DNA recognition motifs, or its binding partners within the PcG and TrxG complexes will reveal new insights into the coordinated epigenetic regulations that is critical to so many fundamental biological processes. In the past year, we have successfully optimized and obtained large, diffraction-quality crystals of the ZH-F1-DNA complex. We have collected X-ray diffraction data of ZH-F1-DNA complex to 2.85 Å. Since there is no suitable known structure that can be used for molecular replacement, we are currently growing heavy-atom derivatives of these crystals in order to solve the phase problem. Crystallization of ZH with PcG and TrxG complexes has already produced small crystals and further optimization is currently underway.

YUHONG WANG, E-1721, University of Houston. THE KINETICS AND CONFORMATIONAL CHANGES DURING THE PEPTIDYL TRANSFERASE REACTION IN SINGLE RIBOSOMES.

1. By applying a novel force-induced remnant magnetization spectroscopy (FIRMS), we have observed the EF-G exerts 89±9 pN force with an effective transition state distance of approximately 0.5 nm. This distance is much less than one codon travelling distance (approximately 2 nm). Therefore, the EF-G is a power-stroke protein at the microscopic scale where the Brownian motion and friction dominate. Our results also provide a method for revealing the general energy coupling mechanism of other motor proteins.

2. We have developed a novel model-free algorithm to reveal the dynamic heterogeneity in the ribosome pre-translocation complex with 2 min interval via the fluorescence resonance energy transfer (FRET) signals in single ribosomes. Different ribosome subpopulations prefer different A-site tRNA configurations, therefore, causing the different profile of the FRET efficiency histograms in individual ribosomes. We have found that the subpopulation

transitions are not random but follow certain pattern. Under the conditions of 20% glycerol or 1 mM viomycin, the transitions are reduced dramatically, indicating the structural fluctuations we observed occur at solvent exposed and inter-subunit locations.

ZHIGAO WANG, I-1827 The University of Texas Southwestern Medical Center. **BIOCHEMICAL IDENTIFICATION OF PROTEASES INVOLVED IN NECROTIC CELL DEATH.**

Toward the first aim, we have shown that overexpression of serpin B8 and serpin B13 significantly protected the cells against necrotic cell death. We then established stable cell lines that expressed tandem-tagged serpin B8 and serpin B13. Tandem immunoprecipitations were performed to identify proteins that specifically bound to serpin B8 and serpin B13 after necrosis induction. So far, we have identified one protease named KLK15 that specifically bound to serpin B13 after necrosis induction. KLK15 is previously reported to be predominantly secreted outside of cell to modify the extracellular matrix. Its role in intracellular proteolysis during necrotic cell death is being actively investigated right now in my lab. At the meantime, we continue to identify more proteases through the tandem immunoprecipitations.

Toward the second aim, we have expressed mammalian mitochondria proteins MFN1 and MFN2 in *E. coli* to be used as substrates for protease activity assay. However, we were unable to detect appreciable protease activity with these substrates. Currently we are trying different protocols to separate intact mitochondria to be used as substrate for protease activity assay. The key is to eliminate lysosome contamination. Immunoprecipitation with Tom20 gave the best outcome. Next we will use that to test in the protease activity assay.

CORAN WATANABE, A-1828, Texas A&M University. ***STREPTOMYCES SAHACHIROI*: A RICH TREASURE TROVE OF UNIQUE BIOSYNTHETIC REACTIONS.**

We completed the synthesis of 5-methylnaphthoic acid and 5-methylnaphthoyl-NAC. These are key compounds needed for evaluation of the PKS. Using the synthetic standard we have unequivocally confirmed the identity of the AziB (PKS)/AziG product as 5-methylnaphthoic acid by LC/MS and LC co-injection. This was an important issue and concern to address as the putative 5-methylnaphthoic acid peak did not match the theoretical mass. It was off by 12 ppm. The compound also resisted fragmentation. We have also confirmed that AziG is the only TE domain of 4 TE domains within the azinomycin gene cluster capable of working in concert with the PKS to generate the azinomycin naphthoate. Active site AziG mutants (E57A, S58A, S61A) and AziB mutant (S1702A) have each been generated. Kinetic and crystallographic studies are now underway.

We also carried out functional knockout of *aziA2* within the azinomycin gene cluster. The gene encodes a NRPS module of unusual domain architecture and leads to overproduction of dimethyl furan 2,4-dicarboxylate, one of many cryptic pathway metabolites from the *S. sahachiroi* genome and is the first non-azinomycin related compound to be isolated from the *S. sahachiroi* strain.

LAUREN J. WEBB, F-1722, The University of Texas at Austin. **THE PHYSICAL CHEMISTRY OF BIOLOGICAL INTERFACES.**

We have made significant progress towards our research objectives this year. We have used our rapidly growing experimental data set to test and refine computational modeling strategies involving molecular dynamics simulations followed by continuum electrostatics calculations to compare our experimental results to theoretical predictions of electrostatic fields. We have demonstrated (Ritchie, *J. Phys. Chem B* 2013) that a highly debated continuum electrostatics calculation can be used to calculate reliable fields under specific and well-defined conditions. We have also demonstrated (Ritchie, *J Phys. Chem B* 2014) that including explicit water molecules in the calculation does not improve the accuracy of the result. We are currently examining more sophisticated computational models, focusing on polarizable (as opposed to fixed-charge) force fields in both the molecular dynamics and electrostatics calculations. We have also significantly expanded our work in measuring the influence of electrostatic fields on the lateral non-covalent organization of lipid bilayer membranes, in particular measuring the effect of cholesterol on the magnitude of fields generated within the bilayer. We have found that this varies based on the composition of the system, and that our results clarify much confusion currently in the literature; we are preparing a manuscript for publication of this work.

R. BRUCE WEISMAN, C-0807, Rice University. **PHOTOSTUDIES OF CARBON NANOSTRUCTURES.**

We have achieved success in a lengthy and challenging project to measure absolute absorption cross sections of different single-walled carbon nanotube (SWCNT) structures. Using a new method, we found sample concentrations by counting many individual nanotubes in near-IR fluorescence microscope images. We determined the first and second optical cross sections of seven SWCNT structures with an estimated accuracy better than 15%. These cross sections are valuable for understanding nanotube electronic properties, and they also enable quantitative sample analysis through simple absorption spectroscopy. A key to this and other advanced studies is access to purified and sorted SWCNT samples. To simplify SWCNT sample preparation, we have developed two novel devices. One uses small permanent magnets to remove nanotube aggregates from dispersed samples, replacing the lengthy ultracentrifugation otherwise needed. The other device is a precise computerized fractionator that delicately extracts purified samples from density gradient ultracentrifuge tubes containing structurally sorted layers. Perhaps our most exciting current project is a new experimental method we call Variance Spectroscopy. Here we use a sensitive apparatus to quickly capture near-IR fluorescence spectra from small volumes of dilute SWCNT samples. Because the probed volume contains a relatively small number of nanotubes, we see significant variations in emission intensity when comparing different spatial regions of the sample. These variations reflect statistical differences in concentration among the probed regions. By analyzing the variations as a function of wavelength over several thousand spectra, we can deduce the abundances of different SWCNT structures, extract their individual (disentangled) emission spectra, and

observe the extent to which they are aggregated in the sample. We think that after suitable development, Variance Spectroscopy will provide a unique and broadly useful bridge between bulk and single-particle spectroscopy.

KENNETH D. WESTOVER, I-1829, The University of Texas Southwestern Medical Center. CHARACTERIZATION OF COVALENT K-RAS INHIBITORS.

We reported the development and characterization of SML-8-73-1 (SML), the first example of a GTP-competitive inhibitor of K-Ras. This included:

- A. Development of an AlphaScreen-based assay to characterize the impact of SML on K-RasG12C:Raf interactions.
- B. Development of hydrogen-deuterium exchange mass spectrometry methods to monitor changes in KRas G12C protein dynamics upon binding of SML to K-Ras G12C.
- C. Solution of high-resolution x-ray structures of K-Ras including G12C and G12C bound to SML.
- D. Application of *in situ* proteomic-based chemical profiling to assess selectivity of SML. This demonstrated that SML is highly selective for K-Ras G12C over other small GTPases.
- E. Development of a novel chemosensor-based assay allowing measurement of covalent reaction rates between K-Ras G12C and SML.
- F. Demonstration using the chemosensor assay that SML can enter the GTP binding site of K-Ras G12C in the context of millimolar concentrations of GTP and GDP, well in excess of what is found in living cells.
- G. Development of a caged version of SML that is cell permeable and exerts effects on the MAPK signaling pathway, albeit at high concentrations.

STEVEN E. WHEELER, A-1775, Texas A&M University. NON-COVALENT π -STACKING INTERACTIONS IN ORGANOCATALYSIS.

We have made tremendous progress in our efforts to understand and quantify the role of π -stacking and other non-covalent interactions on the activity and selectivity of organocatalysts. These efforts are detailed in the five papers published during the previous grant period, as well as several key publications currently in preparation. Most notably, we have re-examined recent claims of "anion- π catalysis" by Matile and co-workers. In contrast to their claims, we have found that anion- π interactions do not contribute to the rate acceleration observed in published examples of this new mode of catalysis. Instead, we show that the net impact of anion- π interactions on these reactions is to increase the activation energy, reducing the reaction rate. However, we were able to computationally design a series of organocatalysts that are predicted to operate and achieve rate acceleration through anion- π interactions.

We have also introduced a new dual-hydrogen-bonding element for hydrogen-bonding organocatalysis. In particular, we have shown that dithiosquaramides, which have never been used in organocatalysis or molecular recognition, provide stronger hydrogen bonds than squaramides, thioureas, or ureas, which are mainstays in the field of hydrogen-bonding catalysis. Moreover, we showed that these dithiosquaramides should provide performance exceeding that of squaramides in a dual-functional organocatalysis for the asymmetric Diels-Alder reactions of nitroalkenes with anthracenes. Recently, there has been independent experimental confirmation by Gale and co-workers (*Chem. Sci.*, 2014, Advance Article, DOI: 10.1039/C4SC01629G) that our dithiosquaramides provide enhanced anion-binding compared to previously available dual-hydrogen-bonding groups.

We have also published other work relating to non-covalent interactions and organocatalysis, including an assessment of the role of π -stacking in a DNA-binding autoantibody, and a study of the enantioselectivity of a primary amine-Brønsted acid catalyzed epoxidation.

MICHAEL A. WHITE, I-1414, The University of Texas Southwestern Medical Center. ANALYSIS OF THE FUNCTIONAL SIGNIFICANCE OF COMPLEX/PROTEIN INTERACTIONS.

Broad-scale mode-of-action annotation of natural product perturbations by Functional Signature Ontology (FuSiOn): A pressing challenge for the biomedical research community is the development of pharmaceuticals that appropriately target newly discovered disease mechanisms. Natural products have proven to be a rich source of bioactive chemicals for medicinal applications but often act through unknown mechanisms and are associated with significant challenges for resupply. To address these challenges we have combined a unique renewable natural products resource with cell-based screening of chemical and genetic perturbations in parallel to return bioactive molecules of interest together with annotation of the cellular components they target. To do this, gene expression-driven functional signatures were employed as cross-platform phenotypic discriminators to link concordant cellular responses to 1124 genetic and 1186 chemical perturbations. Testing of mechanistic hypotheses advanced by the resulting ontology maps expanded molecular annotations of discrete cell biological processes and revealed modes of action and direct protein targets for a variety of novel marine-derived natural products. Specific deliverables include 1) a renewable library of marine-derived bacterial metabolites contains diverse bioactive compounds; 2) a six-gene response signature parses miRNAs, siRNAs, and compounds by cellular activity and mechanism of action; 3) novel genetic and chemical modulators of autophagy, extracellular matrix signaling, and AKT pathway activation; and 4) an open-source data interface to facilitate user-directed queries of chemical and genetic modes of action.

CHRISTIAN P. WHITMAN, F-1334, The University of Texas at Austin. STRUCTURE FUNCTION RELATIONSHIPS IN ENZYMES.

Malonate semialdehyde decarboxylase (MSAD) from *Pseudomonas pavonaceae* 170 is in a bacterial catabolic pathway for the nematocide 1,3-dichloropropene. The enzyme represents one family in the tautomerase superfamily (TSF), which is a model system for the evolution of new enzyme activities. MSAD has two known activities: it catalyzes the metal-ion independent decarboxylation of malonate semialdehyde to produce acetaldehyde and carbon dioxide, as well as the hydration of 2-oxo-3-pentynoate to yield acetylpyruvate. Both activities take place in the same active site using the same groups for binding and catalysis. The purpose of the hydratase activity has never been clear, but it could remove covalent adducts between Pro-1 and reactive aldehydes.

The recent identification and characterization of five new MSAD homologues suggest another possible explanation. Although four of these homologues do not have assigned functions or genomic contexts that indicate functions, a homologue designated Bphy 4401 (or Bp4401) from *Burkholderia phyatum* strain STM815, has a pronounced hydratase activity, converting 2-oxo-3-pentynoate to acetylpyruvate. In fact, the hydratase activity ($k_{cat}/K_m \sim 3 \times 10^3 \text{ M}^{-1}\text{s}^{-1}$) is comparable to that observed for *trans*-3-chloroacrylic acid dehalogenase ($k_{cat}/K_m \sim 6.4 \times 10^3 \text{ M}^{-1}\text{s}^{-1}$), which shows the most robust activity measured for any TSF member thus far. Moreover, there is no detectable MSAD activity. These combined observations suggest that the hydratase activity might reflect a new function in the MSAD family once a biological substrate is identified. The structural and mechanistic bases for this activity are being pursued.

KENTON H. WHITMIRE, C-0976, Rice University. THE CHEMISTRY OF NANOMOLECULES.

In order to probe the effect of solvent and substituents on the formation of $\text{PhBi}(\text{O}_2\text{CR})_2$, BiPh_3 was treated with a variety of carboxylic acids in several solvents. The following were isolated and characterized: $[\text{PhBi}(5\text{-Br-2-OH-C}_6\text{H}_3\text{CO}_2)_2(\text{Me}_2\text{CO})]$; $[\text{PhBi}(5\text{-Br-2-OH-C}_6\text{H}_3\text{CO}_2)_2(\text{EtOH})]$ $(\text{EtOH})(\text{H}_2\text{O})$; $\{[\text{PhBi}(5\text{-O}_2\text{N-2-OH-C}_6\text{H}_3\text{CO}_2)_2(4,4'\text{-bipy})] \text{EtOH} (4,4'\text{-bipy} = 4,4'\text{-bipyridine})$; $[\text{PhBi}(5\text{-Cl-2-NH}_2\text{-C}_6\text{H}_3\text{CO}_2)_2]$; $[\text{Ph}_2\text{Bi}_2(3\text{-MeO-2-OH-C}_6\text{H}_3\text{CO}_2)_4(\text{EtOH})]$; $[\text{Ph}_2\text{Bi}_2(3\text{-MeO-2-OH-C}_6\text{H}_3\text{CO}_2)_4(i\text{-PrOH})]$; $[\text{PhBi}(2\text{-MeC(O)NH-C}_6\text{H}_3\text{CO}_2)_2] \bullet \text{EtOH}$; $[\text{PhBi}(3\text{-MeO-2-OH-C}_6\text{H}_3\text{CO}_2)_2] \bullet \text{PhCH}_3$; $[\text{PhBi}(3\text{-Me-2-NH}_2\text{-C}_6\text{H}_3\text{CO}_2)_2(2,2'\text{-bipy})]$ 0.42MeCN ; $(2,2'\text{-bipy} = 2,2'\text{-bipyridine})$; *cis*- $[\text{PhBi}(5\text{-Br-2-OH-C}_6\text{H}_3\text{CO}_2)_2]_2$; *trans*- $[\text{PhBi}(5\text{-Br-2-OH-C}_6\text{H}_3\text{CO}_2)_2]_2 \cdot 2\text{MeCN}$; $[\text{PhBi}(5\text{-Br-2-OH-C}_6\text{H}_3\text{CO}_2)_2]_2 \cdot 2\text{MeOH}$, *trans*- $[\text{PhBi}(2\text{-OH-C}_6\text{H}_4\text{CO}_2)_2]_2$. Several new structure types were observed including: monomers with a coordinated solvent molecule or a ligand in an equatorial coordination site of a pentagonal pyramidal bismuth(III); asymmetric dimers in which one Bi atom attains the pentagonal pyramidal geometry via coordination a substituent on the carboxylic acid of an adjacent molecule, or dimers in which the carboxylate oxygen atoms themselves are shared reciprocally between the two bismuth atoms. In this last case and both *cis* and *trans* forms are observed. A manuscript on these results is under revision. The new oxo cluster $\text{Bi}_4\text{O}_2(2\text{-OH-C}_6\text{H}_3\text{CO}_2)_8 \cdot 2\text{Solvent}$ was prepared as both MeCN and MeNO₂ solvates. This work has appeared in print as a paper on work done some time ago on In₂O₃ nanoparticles and a new review on Zr and Hf fluoride compounds

KATHERINE A. WILLETS, F-1699, The University of Texas at Austin. CHARACTERIZING SITE-SPECIFIC LIGAND BINDING ON METAL NANOPARTICLE CONJUGATES BY HIGH RESOLUTION FAR-FIELD OPTICAL MICROSCOPY.

Super-resolution fluorescence imaging was used to identify the location of fluorescently-labeled DNA bound to the surface of gold nanorods. In super-resolution imaging, each fluorescent tag on the surface is activated individually and its position determined using a 2-dimensional Gaussian fit. By probing all of the fluorophores on the surface one at a time, the shape and orientation of single gold nanorods is reconstructed, simply by mapping the positions of the labeled ligands bound to the nanorod surface. Many of the nanorods showed significant heterogeneity in where the ligands were bound to the surface, indicating that the fluorescently-labeled DNA does not uniformly saturate the surface, but instead binds preferentially to specific sites along the nanorod. Unfortunately, in all cases, the sizes of the reconstructed nanorods were routinely smaller than they should be. Dipole-based fitting models were developed and used to test whether these models could improve localization accuracy. While the models provided better fits to the diffraction-limited emission of both gold nanorods and surface-enhanced Raman scattering hot spots, this strategy did not improve the reconstructed image size. Additional work on studying local electrochemical potentials on metal nanoparticle electrodes was also performed, revealing site-specific redox potentials based on the location of a single molecule probe on the electrode surface.

RICHARD C. WILLSON, E-1264, University of Houston. PHYSICAL CHEMISTRY OF BIOMOLECULAR RECOGNITION.

We measured the activation energetics of a widely-studied anti-IgE aptamer by anisotropy kinetics over a range of temperatures and ionic strengths, and derived the first (to our knowledge) ever-measured kinetic activation energies and entropies, and changes of these quantities with mutation, for an aptamer/target dissociation process. We extended our single-molecule intramolecular FRET work with C. Landes (Rice University) to characterize the single-site polyelectrolyte adsorption of proteins in unprecedented detail, showing that even chemically-identical sites vary in kinetic properties due to surface entropy and steric effects, and that stochastic clustering dominates conventional adsorption behavior. That work appeared in *PNAS* this spring, and has attracted considerable attention. We have now established the feasibility of similarly studying aptamer/protein association by the measurement of the lifetimes of individual intermolecular complexes. Desorption time distributions observed in the 1-4 Hz observation frequency range are independent of collection frequency and illumination power level, showing the feasibility of investigating this system at the single-molecule level, using a physical observable (binding) orthogonal to the intramolecular FRET we used in our original (and the first) single-molecule investigations of aptamers.

We continue our ¹³C/¹⁵N (DNA and protein) NMR collaboration with A. Pardi (Colorado) on NMR characterization of a specific anti-VEGF aptamer, with the optimal VEGF heparin-binding domain for NMR determined and being produced by the Pardi lab. Finally, we calorimetrically characterized the energetics of recognition of hen egg lysozyme (the canonical model system for structural and physical immunochemistry) by two novel types of molecules selected for specific molecular recognition, nanobodies and affitins, including complexes of known x-ray structure.

C. GRANT WILSON, F-1830, The University of Texas at Austin. PROGRAMMED SELF-ASSEMBLY OF NANOSTRUCTURES.

A process for 3-D programmed self-assembly of lithographically-printable microscale polymer particles using single strand DNA (ss-DNA) hybridization as the associative force was demonstrated. Each of the unit processes required for this approach to self-assembly were demonstrated as was a successful demonstration of the fabrication and sequence-specific self-assembly of covalent single strand DNA-functionalized parallelepipeds with dimensions in the sub-10 μm regime. The assembly was characterized by optical microscopy and imaging flow cytometry.

The major challenge associated with developing this process was in finding a combination of a copolymer, a lift off layer (LOL), immobilization chemistry, a developer, and a stripper that are all mutually compatible. Each working unit operation must be cross-checked with the conditions of the other unit operations in order to be viable. For example, the LOL, must not be appreciably soluble in the copolymer casting solvent, the ssDNA immobilization buffer, the blocking solution, or the developer. Likewise, the stripper for the LOL must not dissolve the copolymer or damage the ssDNA functionalized to the surface.

So, it is possible to pattern the materials, to functionalize one surface with ss-DNA and study the assembly of such particles. The challenge now is to find chemistry that will render these functionalized beads unreactive toward subsequent ss-DNA substitution. This step is crucial for producing the uniquely functionalized surfaces that we require. All attempts to date failed to adequately block the surfaces. Understanding and controlling that chemistry will be the focus the program.

LON J. WILSON, C-0627, Rice University. CARBON NANOCAPSULES AS MRI CONTRAST AGENT PLATFORMS.

Ultrashort single-walled carbon nanotubes loaded with gadolinium ions (gadonanotubes) have been previously shown to exhibit extremely high T_1 -weighted relaxivities ($>100 \text{ mM}^{-1} \text{ s}^{-1}$) To further examine the effect of nanoconfinement on the relaxivity of gadolinium-based contrast agents for magnetic resonance imaging, a series of ultrashort single-walled carbon nanotube (US-tube) materials internally loaded with gadolinium chelates have been prepared and studied. US-tubes were loaded with $\text{Gd}(\text{acac})_3 \cdot 2\text{H}_2\text{O}$, $\text{Gd}(\text{hfac})_3 \cdot 2\text{H}_2\text{O}$, and $\text{Gd}(\text{thd})_3$ (acac = acetylacetonate, hfac = hexafluoroacetylacetonate, thd = tetramethylheptanedione). The longitudinal relaxivities of the prepared materials determined at 25°C in a 1.5 T field were $103 \text{ mM}^{-1} \text{ s}^{-1}$ for $\text{Gd}(\text{acac})_3 \cdot 2\text{H}_2\text{O}@\text{US-tubes}$, $105 \text{ mM}^{-1} \text{ s}^{-1}$ for $\text{Gd}(\text{hfac})_3 \cdot 2\text{H}_2\text{O}@\text{US-tubes}$ and $26 \text{ mM}^{-1} \text{ s}^{-1}$ for $\text{Gd}(\text{thd})_3@\text{US-tubes}$. Compared with the relaxivities obtained for the unloaded chelates ($<10 \text{ mM}^{-1} \text{ s}^{-1}$) as well as accounting for the T_1 reduction observed for the empty US-tubes, the boost in relaxivity for chelate-loaded US-tubes is attributed to confinement within the nanotube and depends on the number of coordinated water molecules

LANI F. WU, I-1644, The University of Texas Southwestern Medical Center. ON THE EVOLUTION OF DRUG-RESISTANT LUNG CANCER SUBPOPULATIONS.

Over the past two years, we pursued an approach for isolating and studying clonal populations under the selective pressure of the EGFR-inhibitor erlotinib. Our approach removes the sampling bias for the fittest subpopulations and allows us to investigate diverse survival mechanisms used by small subpopulations that could be dominant in the context of other selective pressures.

We began with a clonal PC9 population, grown in $2.5 \mu\text{M}$ erlotinib, a dose 100-fold in excess of the cell line's IC_{50} for erlotinib and comparable to the dose that lung adenocarcinomas are exposed to when treated in the clinic- Drug-resistant clones of PC9-I were then derived in physical isolation, and selected for their ability to proliferate in the presence of erlotinib. Initial observations revealed clone-to-clone differences in cell size, morphology, growth kinetics, and signaling. Today we have generated seventeen of these drug resistant clones.

We assessed whether these erlotinib-resistant clones would revert their original parent drug sensitivity upon the removal of the erlotinib treatment. We monitored these clones over a period of forty weeks and we found that only one of our seventeen drug resistant clones reverted to the same levels of erlotinib sensitivity as the parent. The sixteen clones either remained completely resistant to erlotinib or reverted to approximately half the sensitivity of the parent. Our results are quite interesting. First, previous studies showed complete reversion to sensitivity, suggesting epigenetic mechanisms of resistance, which our clones do not appear to have. Second, our clones do not appear to have the most common known mechanisms of genetic resistance as based on sequencing results of the EGF receptor. We are now pursuing both a genetic and pharmacological strategy for identifying mechanisms underlying the observed resistance.

ROBERT E. WYATT, F-0362, The University of Texas at Austin. COMPUTATIONAL INVESTIGATION OF ELECTRON DYNAMICS IN LIGHT-MATTER INTERACTIONS.

During the past year, progress has been made on three research projects. (1) Numerical variance reduction for Monte Carlo dynamics. Due to autocorrelations inherent in the data, Markov chain Monte Carlo simulations yield distributions of computed properties with large variance. A new method has been developed to transform the raw data so that the variance is reduced significantly. The method has been applied to data from lattice quantum field computations in elementary particle physics and leads to more reliable estimates of physical properties such as energy and mass. (2) Relativistic ionization dynamics with intense laser pulses. An efficient parallel computer code has been developed to simultaneously integrate the relativistic Dirac equation and Maxwell's equations for attosecond pulse ionization of hydrogenic atoms. Production runs will begin soon and animations showing the time dependence of Dirac spinor components during the ionization process are expected to be very insightful. (3) New approach to computation of real-time Feynman path integrals. Path integrals are notoriously difficult to compute due to rapid oscillations of the integrand. A new approach has been developed to mitigate difficulties inherent in traditional approaches. After introducing a spatial filter to dampen high frequency oscillations, hyperspherical coordinates are introduced. Following Monte Carlo selection of the hyper-angles, one-dimensional radial integrals are accurately evaluated using grid methods. Applications have been made to problems in quantum dynamics, including quantum field theory (specifically, scalar spin-0 particles, such as the Higgs boson), an area noted for the absence of real-time dynamical studies.

MIGUEL JOSE YACAMAN, AX-1615, The University of Texas at San Antonio. CONTROLLING THE SHAPE AND PARTICLES USING WET CHEMISTRY METHODS: THE CASE OF BIMETALLIC NANOPARTICLES.

During this period the work was focused on two aspects: start to analyse Trimetallic particles and to go in deep in one particular case of bimetallic the Au/Cu. The rationale of studying three metals is that we gain more control of the chemistry of the particle. An important result was obtained on the Au/Pd/Pt system. We found that we could induce all the platinum metal to be on the surface. That opens the possibility of optimizing catalysts for fuel cells that are intensive on Pt and therefore very expensive and difficult to make it commercial.

In the case of bimetallic we concentrate our efforts on Au/Cu. This system is very interesting from the scientific point of view and was the base of the old Corinthian Bronze which was some of the most important materials of antiquity. This alloy is very rich on properties. However the rules of the bulk alloys are not necessary valid for the nanoscale. That is why it is necessary to find out how we can mimic the bulk alloys.

Our work this year resulted in the following.

Two PhD thesis completed on the topic. The students were: Nabraj Bhattarai with the dissertation SYNTHESIS AND ELECTRON MICROSCOPY CHARACTERIZATION OF BIMETALLIC NANOPARTICLES AND ATOMICALLY CONTROLLED Au NANOCCLUSERS and Subarna Khanal with the thesis ADVANCED ELECTRON MICROSCOPY CHARACTERIZATION OF MULTIMETALLIC NANOPARTICLES.

We published eight papers that acknowledge the grant.

We trained fifteen undergrad students and we have four new students working on their PhD in the lab.

We organized a workshop on electron microscopy of nanostructures in January 2014.

BORIS I. YAKOBSON, C-1590, Rice University. SCIENCE OF NEARLY-1D MATERIALS: FROM NANOTUBES TO NANOWIRES.

During the previous/first year of this grant we continued our 2D and 1D-materials studies, including the fundamental growth mechanisms (e.g. graphene on Cu, and the role of hydrogen promoter), as well as emerging imbedded-1D structures of general importance: 1D grain boundaries (GB) in transition metal dicalcogenides (MS_2), including GB dynamics and ferromagnetism. We have extended our study of carbyne $[...C\equiv C...]_n$ as ultimate monoatomic wire, where we determined the stiffness and strength and further discovered/predicted metal-insulator transition induced by mechanical tension. Following the earlier years experiences with electronic transport, we computed conductance through various nanotube junctions, both the quantum details of single junctions and collective percolation phenomena in the array-fibers. Our scope of selected nanostructures remains intentionally broad as we aim to identifying the common physico-chemical features in both formation/synthesis and functionality.

NAN YAN, I-1831, The University of Texas Southwestern Medical Center. TAIL-ANCOR OF A CRITICAL INNATE IMMUNITY REGULATOR TREX1 ON THE ER.

During the first project year, we have made progress on all aims. We have determined that TREX1 is localized to the ER through the TRC40 tail anchor pathway. More specifically, we have demonstrated that TRC40 is required for TREX1 localization to the ER, and TREX1 interacts with TRC40 biochemically through the C terminal end that harbors the predicated hydrophobic region. We also found that siRNA knockdown of TRC40 or deletion of the TREX1 hydrophobic region mislocalized TREX1. We have also explored the function of TREX1 tail-anchoring on the ER and found a novel connection to the ER glycosylation machinery. Below is the abstract of a manuscript we recently submitted to Nature Medicine.

TREX1, also known as DNase III, is an endoplasmic reticulum (ER)-associated negative regulator of innate immunity. Human TREX1 mutations are associated with a spectrum of autoimmune and inflammatory phenotypes, and accumulated self-DNA is thought to be a trigger of disease. However, since many TREX1 disease-causing mutations mislocalize TREX1 within the cell without disrupting DNase activity, it is unclear how they cause autoimmunity. Here we show that TREX1 is a tail-anchored (TA) protein that localizes to the ER through the mammalian TRC40 TA pathway. Using *Trex1*^{-/-} cells reconstituted with representative TREX1 mutants, we found that TREX1 ER membrane anchoring, but not DNase activity, regulates cell-intrinsic activation of immune genes. In addition, *Trex1* unexpectedly suppressed a widely-known yet enigmatic hydrolytic process that liberates mannose-rich free glycans from ER membrane-associated dolichol-linked oligosaccharides into vesicular compartments. Hydrolysis in *Trex1*^{-/-} cells is prevented by expressing wild type or DNase-inactive TREX1, but not mislocalized (DNase active) TREX1. Similarly, we detected free glycan accumulation in skin fibroblasts from an individual with systemic lupus erythematosus carrying the P212fs mislocalization mutation but not from fibroblasts carrying wild type or DNase-dead D18N TREX1. We further found that free glycans from TREX1^{-/-} cells induced an immune gene signature in wild type cells matching that of *Trex1*-deficiency. Together our data reveal a new DNase-independent function of TREX1 that suppresses liberation of free glycans with potential to provoke a sterile immune response. This new function may help account for autoimmune disease associated with mislocalization of DNase-active TREX1.

JIONG YANG, A-1700, Texas A&M University. DEVELOPMENT OF NEW REAGENTS FOR SELECTIVE ENOLIZATION OF CARBONYL COMPOUNDS.

Building upon our preliminary studies of the previous funding period, our research during this funding period focused on developing synthetic methods based on iron-catalysis because of the unique reactivity of iron compared with other transition metals, the high abundance of iron in the Earth's crust, and the low toxicity of most iron salts. We successfully developed a number of low-valent iron-catalyzed transformations. Firstly, we developed a low-valent iron catalyzed protocol for reductive cyclization of unactivated 1,6-enynes. This transformation made use of a combination of diethylzinc and magnesium(II) bromide etherate for converting iron(II) chloride into the catalytically active species in the presence of an alpha-iminopyridine ligand. Compared with existing methods, this protocol is practical because no air-sensitive organoiron complexes have to be isolated and this reaction does not require transition metals that are

expensive or toxic. Secondly, we developed an iron-catalyzed intermolecular hydroamination reaction. The catalytically competent organoiron species, formed by a combination of iron(II) chloride, cyclopentylmagnesium bromide, and the alpha-iminopyridine ligand, enabled the intermolecular hydroamination of styrenes using electrophilic *O*-hydroxylamine esters. To the best of our knowledge, this transformation represents the first example of iron-catalyzed hydroamination of alkenes using electrophilic nitrogen sources. We also explored iron-catalyzed C-H functionalization during this funding period.

FELIX YAROVINKSY, I-1799, The University of Texas Southwestern Medical Center. THE STRUCTURAL BASIS OF PARASITE RECOGNITION BY TRL11 AND TRL12 RECEPTORS.

During last year we have solved structures of *Toxoplasma gondii*, *Plasmodium falciparum*, and *Cryptosporidium parvum* profilins. We have also applied site directed mutagenesis studies and mapped the active site on profilin proteins that are responsible for activation of TLR11 and TLR12. Additional biochemical experiments established all molecules that are involved in the TLR11 and TLR12 signaling complex: TLR11- profilin (1:1 ration) establish a heterodimer with TLR12 bound to profilin (1:1 ratio), MyD88 interacting with TLR11 (but not TLR12), and UNC93B1 that interacts with both TLR11 and TLR12. We have also expressed TLR11 and TLR12 ectodomains in quantities sufficient for crystallization.

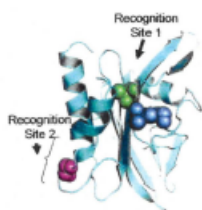


Figure 1. *T. gondii* profilin residues interacting with TLR11. Our binding and site-directed mutagenesis experiments identified two sites in the N-terminal domain of profilin are recognized by TLR11: G16, A26, and K44

JIN YE, I-1832, The University of Texas Southwestern Medical Center. SATURATED FATTY ACID-INDUCED LIPOTOXICITY

We have previously identified Ubx8 as an intracellular sensor for fatty acids that initiate various reactions maintaining fatty acid homeostasis in mammalian cells. The selective interaction of Ubx8 to unsaturated but not saturated fatty acids may explain some toxic effects of saturated fatty acids. During the past year we identified the UAS domain within Ubx8 as the motif interacting with unsaturated fatty acids. This finding suggests that proteins containing the UAS domain may be regulated by unsaturated fatty acids. Indeed, we found that excess unsaturated fatty acids may facilitate proliferation of certain cancer cells by inhibiting FAF1, a tumor suppressor that contains the UAS domain.

During the past year we also identified another mechanism through which saturated fatty acids trigger lipotoxicity. We found that increased ratio of saturated to unsaturated fatty acids inhibited the reacylation reaction of phospholipids in the Land's cycle, resulting in accumulation of lysophosphatidylcholine (LPC). The accumulation of LPC in turn triggered ER stress, which has been implicated as the underlying mechanism for lipotoxicity in multiple organs.

DANNY L. YEAGER, A-0770, Texas A&M University. DEVELOPMENTS AND STUDIES USING SEVERAL COMPLEX SCALED MULTICONFIGURATIONAL METHODS FOR ELECTRON ATOM/MOLECULE RESONANCES.

Electron-atom/molecule resonances are temporarily bound states which lie in the continuum part of the Hamiltonian. If the electronic coordinates of the Hamiltonian are scaled ("dilated") by a complex parameter, $\eta = ae^{i\theta}$ (a, θ real), then its complex eigenvalues represent the scattering states (resonant and non-resonant) while the eigenvalues corresponding to the bound states and the ionization and the excitation thresholds remain real and unmodified. These make the study of these transient species amenable to the bound state methods.

The complex scaled multiconfigurational time-dependent Hartree-Fock method (CMCTDHF also called the complex scaled multiconfigurational linear response method (CMCLR)) has been used to study the doubly excited He $2s^2$ Feshbach resonance energy and lifetime. Various even-tempered Gaussian basis set/complete active space (CAS) combinations are examined. The results are compared with the complex scaled full CI, cs-EOM-CCSD methods and exact numerical calculations. It was shown that CMCTDHF is able to provide highly accurate resonance parameters with a fairly tractable size of basis set and CAS, where the computational resources required are much less than full CI or cs-EOM-CCSD methods and exact numerical results.

HSIN-CHIH YEH, F-1833, The University of Texas at Austin. NANOCUSTER BEACONS FOR HIGH SPECIFIC DNA METHYLATION DETECTION.

With the Welch support, we have written two review papers. One entitled "fluorescent silver nanoclusters as DNA probes" was published in *Nanoscale* (2013, 5, 8443-8461), which cited more than 200 papers in its references. These reviews will help promote the widespread use of silver clusters as new fluorescent labels in analytical chemistry and quantitative biology. Our NanoCluster Beacons have many advantageous properties. Recently we have discovered the rules (e.g. through systematical modification of the nucleation sequences) to tune the emission colors of NanoCluster Beacons and successfully extended NanoCluster Beacons into multicolor, activatable probes. A manuscript about this work has been submitted to *ACS Nano* and is currently under review. Understanding the key factors that determine the emission colors of NanoCluster Beacons are critically important for using NanoCluster Beacons in DNA methylation detection. Other researchers can also take advantage of our discoveries in designing new sensors to detect other molecules of their interest.

We are moving toward the DNA methylation detection (5mC or 6mA) based on the multicolor NanoCluster Beacons. We continue to make progress in understanding the chemical and photophysical properties of this emerging fluorophores. With the Welch support, I have also networked and formed collaborations with important silver cluster researchers in the world, such as Jeffrey Petty at Furman University, Seong-Wook Yang and Tom Vosch at University of Copenhagen.

SHERRY J. YENNELLO, A-1266, Texas A&M University. THE EQUATION OF STATE FOR A TWO-COMPONENT NUCLEAR SYSTEM.

A nucleus in its ground state can be viewed as a liquid drop composed of two different components - protons and neutrons. Isospin asymmetry is a measure of the neutron - proton imbalance. When a nuclear collision happens kinetic energy is converted into excitation energy thus heating the nuclear material. As the nuclear material is heated and cooled it explores the equation-of-state of this two-component system. The mechanisms by which nuclei collide, equilibrate and fragment are dependent on the isospin asymmetry. By investigating the reactions of nuclei that vary in isospin asymmetry we can elucidate the underlying reaction mechanisms and their dependence on isospin. In order to carry out this program a new experimental apparatus was constructed, the quadrupole triplet spectrometer (QTS). The QTS magnetically separates the projectile-like fragments from the unreacted beam (which is stopped in a faraday cup at zero degrees) and focuses them on a silicon detector 7.5 m downstream. The FAUST detector array was coupled to the QTS to measure the light charged particles, detected in FAUST, in coincidence with the projectile-like fragments, measured with the QTS. We utilized this new experimental setup to investigate the reaction mechanism competition from the reactions of ^{136}Xe and ^{124}Sn with ^{64}Ni and ^{124}Xe with ^{58}Ni at 15 Mev/nucleon to produce heavy 3-body breaking of the reacting system. It has been proposed that the isospin content, alignment and velocity distributions of these fragments represent observables sensitive to the nuclear equation of state.

HYE-JEONG YEO, E-1616, University of Houston. STRUCTURAL STUDIES OF NOVEL SURFACE POLYPEPTIDES.

Bacterial lipoproteins are universal components of bacterial membrane and have diverse functions including cell adhesion, transport, nutrient acquisition, and stimulation of inflammatory immune responses in host cells. Our recent crystal structure of Cj0090 (specific aim 1) at 1.9 Å resolution revealed a novel variant of the immunoglobulin (Ig) fold with β-sandwich architecture, suggesting a possible role for the cell surface lipoprotein Cj0090 in protein-protein interactions. A recent study showed that Cj0090 was expressed as a three-gene operon (*cj0089*, *cj0090*, and *cj0091*) encoding a cluster of lipoproteins in *C. jejuni*. This operon appears to be subject to direct regulation by CmeR, a transcriptional regulator repressing the expression of the multidrug efflux pump CmeABC. We aimed to unravel the structure-function relationship of these three proteins. We found that Cj0091 was localized at the outer membrane, supporting a role of Cj0091 in lipoprotein-mediated adherence. We have cloned and expressed two other genes in the operon, *cj0089* and *cj0091*. We made progress on protein purification for crystallization of these two proteins. Our structural and biochemical characterization will establish the specific roles of the lipoprotein cluster in the adhesive activity of *C. jejuni*.

GANG YU, I-1776, The University of Texas Southwestern Medical Center. ATOMIC STRUCTURE AND MECHANISM OF THE γ-SECRETASE COMPLEX.

γ-Secretase is an intramembrane protease complex of Presenilin, Pen-2, Aph-1, and Nicastrin. It proteolyzes the precursor protein for Alzheimer-linked amyloid-β peptides. During the past year, my collaborators and I have continued our efforts to solve high-resolution structures of Nicastrin and the whole γ-secretase complex. We have made steady progresses in our endeavors in using X-ray crystallography for structural studies of γ-secretase. We have also initiated efforts to take advantage of the recent advances in cryo-EM techniques. We refined our experimental constructs, systems and approaches, produced additional tools such as conformational specific antibodies, and initiated multiple crystallization trials. However, despite intensive efforts, we have not yet been able to obtain high-quality crystals of human γ-secretase complex and its components. On the biochemical front, we have extended our analysis for a role of Nicastrin as a substrate recognition subunit and for how γ-secretase is activated via a secondary folding mechanism. The recent report of a 4.5 Å cryo-EM structure of γ-secretase provided strong support for our models of γ-secretase assembly and architecture, and of Nicastrin as a substrate receptor. It was shown that the Nicastrin ectodomain resembles an aminopeptidase, containing a large lobe and a small lobe. The large lobe contains a substrate-binding pocket, as we previously proposed, that is 60 Å away from the membrane embedded catalytic site, ideal for accommodating the N-terminal stub of a substrate. We have performed additional computational modeling based on this structural information to help interpret our preliminary (unpublished) biochemical data and refine the design of additional experiments. Thus, despite a lack of an atomic structure of the γ-secretase complex, we have made inroad towards a mechanistic understanding of γ-secretase.

HONGTAO YU, I-1441, The University of Texas Southwestern Medical Center. BIOCHEMICAL AND STRUCTURAL ANALYSIS OF SISTER-CHROMATID COHESION.

Timely establishment and removal of sister-chromatid cohesion are critical for the fidelity of chromosome segregation. Dysregulation of these processes causes aneuploidy, a driver of tumorigenesis and other human diseases. Sister-chromatid cohesion requires the cohesin complex, which consists of Smc1, Smc3, Scc1, and SA2 in humans and forms a ring-like structure. Cohesin binding to chromatin is dynamically controlled by both positive and negative regulators. Wap1 is an anti-establishment factor for cohesin and catalyzes the removal of cohesin from chromatin. During S phase, Smc3 acetylation enables the binding of sororin to the cohesin cofactor Pds5, which protects cohesin from Wap1, thus establishing functional cohesion. In mitosis, shugoshin (Sgo1) in complex with protein phosphatase 2A (PP2A) protects cohesin from mitotic kinases and Wap1 at centromeres to prevent premature chromosome segregation. In the past year, we have determined the crystal structure of human SA2 bound to the central region of Scc1. We further show that Sgo1 and Wap1 compete for

binding to a conserved site on SA2–Scc1. Thus, Sgo1 physically shields cohesin from Wap1. This unexpected, direct antagonism between Sgo1 and Wap1 augments centromeric cohesion protection.

YONGHAO YU, I-1800 The University of Texas Southwestern Medical Center. LARGE-SCALE ISOLATION AND IDENTIFICATION OF POLY-ADP-RIBOSYLATED PROTEINS.

We have established a state-of-the-art mass spectrometry platform that allows us to perform large-scale analyses of the ADP-ribosylated proteome (protein ADP-ribosylation is a posttranslational modification that is catalyzed by a family of enzymes termed PARP). Using high resolution mass spectrometry, we characterized the human Asp- and Glu-ADP-ribosylated proteome and identified 1,048 ADP-ribosylation sites on 340 proteins that were involved in a wide array of nuclear functions. In addition, we have, within last year, adapted this pipeline for quantitative analysis of protein ADP-ribosylation. This is a significant achievement, because this platform now allows us to analyze the change in the ADP-ribosylated proteome upon the treatment of PARP inhibitors. Indeed, using this technology, we identified hundreds of novel PARP downstream effector proteins. PARP inhibitors are a class of compounds that have shown great promise in the clinic. In particular, late stage clinical trials have indicated that a subpopulation of (specifically, *BRCA*-deficient) breast cancer and ovarian cancer patients show dramatic responses to PARP inhibitors. We envision that the identification of these novel PARP substrates will greatly facilitate the understanding of not only the biology of protein ADP-riboseylation, but also how to better utilize PARP inhibitors to treat human cancer.

ANVAR A. ZAKHIDOV, AT-1617, The University of Texas at Dallas. PHOTOCHEMICAL REACTIONS IN DYE SENSITIZED SOLAR CELL WITH BISCROLLED GRAPHENE QUANTUM DOT ELECTRODES.

We demonstrated an organic photovoltaic (OPV) device with an electrochemically gated carbon nanotube (CNT) charge collector. Bias voltages applied to the gate electrode reconfigure the common CNT electrode from an anode into a cathode which effectively collects photogenerated electrons, dramatically increasing all solar cell parameters to achieve a power conversion efficiency of ~3%. This device requires very little current to initially charge and the leakage current is negligible compared to the photocurrent. This device can also be viewed as a hybrid tandem OPV-supercapacitor with a common CNT electrode. Other regimes of operation are analysed.

We demonstrated the effects of nanostructure geometry on the nanoimprint induced poly-(3-hexylthiophene-2,5-diyl) (P3HT) chain alignment and the performance of nanoimprinted photovoltaic devices. Out-of-plane and in-plane grazing incident X-ray diffraction techniques are employed to characterize the nanoimprint induced chain alignment in P3HT nanogratings with different widths, spacings and heights. We observe the dependence of the crystallite orientation on nanostructure geometry such that a larger width of P3HT nanogratings leads to more edge-on chain alignment while the increase in height gives more vertical alignment. Consequently, P3HT/[6,6]-phenyl-C61-butyric-acidmethyl-ester (PCBM) solar cells with the highest density and aspect ratio P3HT nanostructures show the highest power conversion efficiency among others, which is attributed to the efficient charge separation, transport and light absorption. This work has been highlighted by NanoWerk in the article by Michael Berger.

Semitransparent Polymer Light Emitting Diodes (PLEDs) with double side emission using Multiwall Carbon Nanotubes (MWCNT) sheets as top transparent cathode are described. The combination of an effective electron injection layer and a hole blocking layer: PFN/Cs₂CO₃, allowed an enhancement of the electron injection from the MWCNT sheets. Those semitransparent devices exhibited a brightness and an efficiency of 220 Cd/m² and 0.54 cd/A respectively, which were measured on the glass side. Our results indicate that the new architecture of laminated top-MWCNT could be useful for the development of transparent displays using a vacuum free simple dry fabrication process.

CHENGCHENG ZHANG, I-1834, The University of Texas Southwestern Medical Center. SMALL MOLECULE MODULATORS OF ANGPTL RECEPTOR FOR STEM CELL EXPANSION AND LEUKEMIA TREATMENT.

In Aim 1, we already identified a number of small molecule chemicals that block a downstream signaling pathway of LILRBs. The blocking effects of the LILRB antagonists were validated by *in vitro* enzymatic assays and *in vivo* cellular reporter system. We have not identified agonists of the receptor signaling yet.

In Aim 2, we showed that two of these identified compounds efficiently induced apoptosis of a number of human leukemia cell lines *in vitro* and decreased colony forming ability of primary mouse AML stem cells. The toxicity to normal HSCs is significantly less based on the same assay. Importantly, we found these two chemicals delayed leukemia development in the mouse model of acute myeloid leukemia.

CHUN-LI ZHANG, I-1724, The University of Texas Southwestern Medical Center. BIOCHEMICAL REGULATION OF THE ORPHAN NUCLEAR RECEPTOR TLX.

Through the regulation of intracellular signaling pathways or direct control of transcription factor activities, small molecules may exert fundamental impact on cell behavior and fate. We recently showed that the small molecules forskolin (FSK) and dorsomorphin (DM) can facilitate the transcription factor NGN2 to very efficiently reprogram human fetal fibroblasts to cholinergic neurons. When additional transcription factors are added, these molecules can also convert adult human skin fibroblasts to cholinergic motor neurons. These induced motor neurons (iMNs) can form functional synaptic connections with cocultured cortical neurons and can form neuromuscular junctions and control muscle contraction when cocultured with mouse myotubes. Most importantly, iMNs can also be derived from human patient skin fibroblasts with amyotrophic lateral sclerosis (ALS). The iMNs from ALS patients are defective in the formation of neuromuscular junctions and the control of muscle contraction. Most importantly, these iMNs survived worse than those from healthy control

patient fibroblasts. A functional screen will be conducted in the near future to identify small chemical compounds that will promote survival and growth of ALS-iMNs. These small molecules might have therapeutic values for treating ALS patients.

We also examined the molecular mechanism underlying small molecule-mediated reprogramming of human fibroblasts. As NGN2 activity is controlled by phosphorylation, we first examined whether this modification plays a critical role during cellular reprogramming and found that it is not essential. We then performed systematic and unbiased experiments through RNA-seq and ChIP-seq under conditions with small molecule- or vehicle-treatment. These results will reveal global changes on transcriptional activity and chromatin association of transcription factors. Future work will be to understand how small molecules induce global changes that can ultimately lead to cell fate switch.

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 hydrocarbon oxidation reactions initiated by the hydroxyl radical (OH) and ozone (O₃). Progress has been made in laboratory studies of the oxidation of biogenic (isoprene and α -pinene) and anthropogenic (toluene) hydrocarbons, focusing on the product yields and their contributions to formation and transformation of secondary organic aerosol. Using an environmental chamber, we have simulated the OH-initiated oxidation of isoprene, α -pinene, and toluene and assessed their roles in atmospheric aging of primary particles. Size-classified soot aerosols are introduced into the environmental chamber in the presence of hydrocarbons, photolytically generated OH, O₃, and nitrogen oxides. The evolution in the mixing state of soot particles is monitored from simultaneous measurements of the particle size and mass, which are used to calculate the particle effective density, dynamic shape factor, mass fractal dimension, and coating thickness. Our results suggest that ubiquitous biogenic and anthropogenic hydrocarbons play an important role in aging of primary aerosols, shortening their atmospheric lifetime and considerably altering their impacts on air quality and climate. In addition, the interaction between dimethylamine and organic acids is investigated using Basin Paving Monte Carlo (BPMC) sampling with the classical force field to obtain low energy conformers of dimethylamine and succinic acid hydrated molecular clusters. Geometry optimization and frequency calculations are further performed on the basis of the BPMC results using density functional theory. The free energies of formation for hydrated clusters consisting of dimethylamine and succinic acid reveal that the interaction between amines and dicarboxylic acids likely exerts a synergetic effect on atmospheric aerosol nucleation by formation of aminium carboxylate ion pairs.

XIUREN ZHANG, A-1777, Texas A&M University. BIOCHEMICAL BASIS OF *ARABIDOPSIS* ARGONAUTE 10 AS A DECOY FOR microRNAs.

We have previously focused on Aims 1 and 2 (Investigate the binding capacity of AGO10 as a decoy for miR166/165 and Determine the biochemical basis of AGO10 for its decoying capacity for miR166). We performed a series of domain-swapping experiments between AGO1 and AGO10 and found that their N-terminal domains grant their functional specificity. We have successfully completed these missions. More than that, we have also explored the biochemical mechanism of miR166 processing in *Arabidopsis*.

To further extend our research the unique function and regulation of AGO10-miR166, we have recently applied mosaic silencing technology to knockdown miR166 in particular tissues and developmental stages. We found that AGO10 represses miR165/166 activity in a range of regions emanating from embryo proper in the early embryogenesis, to the apical and central regions of the mature embryos, and eventually to the entire adaxial domains and vasculature tissues in the cotyledons and leaf primordia. These locations are essentially identical to the accumulation domains of *PHABULOSA* and *REVOLUTA* transcripts that are targeted by miR165/166. *Arabidopsis* genome contains nine *MIR165/166* genes. Sequestration of miR165/166 through the promoters of *MIR165b*, *MIR166a*, *MIR166b* and *MIR166g*, but not other members, efficiently rescued the SAM defect in *ago10* mutants. Comparison of the expression patterns of *AGO10* and the four *MIR165/166* members suggested the AGO10 quenches the non-cell-autonomous activity of miR165/166 that are produced outside and diffused into *AGO10*-confined niches. Thus, this study provides new insight into how the spatiotemporal regulation of the AGO10-miR165/166 activity affects the SAM development.

XUEWU ZHANG, I-1702, The University of Texas Southwestern Medical Center. AUTOINHIBITION OF PLEXIN BY A NEW CONFORMATION-MEDIATED DIMER.

In the past year, we have established a collaboration with Dr. Adam Smith (U. of Akron) to perform Pulsed-Interleaved Excitation Fluorescence Cross-Correlation Spectroscopy (PIE-FCCS) experiments to probe the preformed dimer of plexin on the cell surface. The results demonstrate that plexin is predominantly dimeric on the cell surface prior to semaphorin binding. The extracellular Sema domain is required for formation of this inhibitory dimer, while the intracellular domain may contribute to its stability. Our data show that semaphorin binding activates plexin by switching it from the inhibitory dimer to the active dimer. We will introduce structure-based point mutations to probe the interfaces of both dimers in detail. Once these experiments are completed, a paper on the inhibitory dimer of plexin will be published, which will establish a major functional state of plexin in cell signaling. Our goal in the next three years will be focused on the specific interaction between plexin and two guanine nucleotide exchange factors (GEFs) PDZ-RhoGEF and LARG, which play essential roles in plexin signaling. It has been shown that these GEFs use their PDZ domains to bind the C-terminal tail of class B plexins. We have solved a crystal structure of a class B plexin in complex with the PDZ domain of PDZ-RhoGEF. The structure reveals an additional interface between plexin and the PDZ domain, which likely underlies the unexplained high degree of specificity between the two. We will perform biophysical measurements and cell-based assays to test whether the secondary interface is indeed important for the specific binding *in vitro* and plexin signaling inside the cell.

YAN JESSIE ZHANG, F-1778, The University of Texas at Austin. CHEMICAL SENSORS TO DETERMINE PROLINE ISOMERIC SPECIFICITY OF RNA POLYMERASE II.

The post-translational modification (FTM) states of the unique structure of RNA Pol II at C-terminal domain have been found to be correlated to different stages of transcription. The interpretation of the biological implication of such PTM states are further complicated since there seems to be cross-talk between different sites. Prolyl isomerization is particularly difficult to study due to the lack of direct and simple method to establish the prolyl isomerization selectivity of CTD enzymes. Herein, we incorporated locked prolyl isosteres analogues as surrogate for proline residues following Ser2 and Ser5 in CTD consensus sequence. This design allows us to determine the prolyl selectivity of CTD phosphatases: Ssu72 as cis-specific, Scp1 and Fcp1 with strong preference towards trans proline. Due to this prolyl selectivity, enzymes like human Pin1 that can speed up cis:trans conversion show differentiated effect on these phosphatases and therefore results in different effect on the phosphatase activity of the CTD phosphatases. These effects are physiologically relevant and have direct impact on different CTD modification sites *in vivo*. Our research developed chemical compounds that can be used to determine the proline isomeric selectivity of proteins and used it to understand the regulatory mechanism for transcription.

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, we continued our investigation on applying the self-assembled modularly designed organocatalysts (MDOs) in asymmetric catalysis and synthesis, as proposed in our proposal. We have achieved a high stereoselective Mannich reaction using the MDOs. Most importantly, we have realized highly diastereodivergent catalyses with these MDOs. One manuscript on the tandem Michael-Michael reaction is now published in *Angew. Chem. Int. Ed.*, in which we realized the synthesis of eight of the sixteen possible (half set) stereomers from the same substrates in excellent stereoselectivities (up to >99:1 dr and >99% ee). The method was also demonstrated to be very useful for the synthesis stereoisomeric natural products. Diastereodivergent catalysis is an emerging area of research in asymmetric catalysis since there are only a handful of examples reported so far in the literature. According to our preliminary data, MDOs are perfect catalysts for this purpose since the method developed in our lab is quite general: two other diastereodivergent catalytic methods are almost completed by now and additional ones are in the working. We also continued on the study of the enolate-mediated organocatalytic asymmetric reactions. In this area, we published three papers and one additional paper was recently submitted. One of these papers was highlighted as a cover picture. In addition, we continued our collaborations with Dr. Chen, which resulted in two publications and one submitted manuscript. One of the methods we developed using the MOF provided by Dr. Chen was highlighted by *Synfacts*. One more manuscript is currently under preparation and will be submitted soon. We also made five presentations at local and national conferences in which we acknowledged the financial support of the Welch Foundation in the past year.

ALEKSEI M. ZHELTIKOV, A-1801, Texas A&M University. OPTICAL DETECTION OF ULTRAFAST ELECTRON DYNAMICS AND ELECTRON-INITIATED CHEMICAL PROCESSES.

A closed-form solution has been found for the nonadiabatic ionization rate in a transparent dielectric medium, revealing ultrafast ionization dynamics within the field cycle and recovering the key results of the earlier photoionization theories in the appropriate limiting regimes. An ultracompact fiber-optic probe was designed and demonstrated as a part of our research program with a diamond microcrystal attached to the fiber tip, allowing the electron spins of nitrogen-vacancy (NV) centers to be manipulated, polarized, and read out through a fiber-optic waveguide integrated with a two-wire microwave transmission line. The microwave field transmitted through this line is used to manipulate the orientation of electron spins in NV centers. The electron spin is then optically initialized and read out, with the initializing laser radiation and the photoluminescence spin-readout return from NV centers delivered by the same optical fiber. A specifically designed implantable fiber-optic interface for parallel long-term optical interrogation of distinctly separate, functionally different sites in a living brain has been also demonstrated. Two-photon excitation has been shown to substantially enhance the locality of fiber-based optical interrogation of strongly scattering biotissues. Fiber probes with a high numerical aperture and a large core area are shown to enable locality enhancement in fiber-laser-fiber-probe two-photon brain excitation and interrogation without sacrificing the efficiency of fluorescence response collection. The theory of photoionization in a dielectric medium has been generalized to the case of arbitrarily short driving pulses. Combining advanced ultrafast laser technologies with novel methods of nonlinear-optical waveform characterization, we extended time-domain spectroscopic techniques to an ultrafast detection and diagnostics of fundamental molecular motions in the mid-infrared spectral range.

JUNRONG ZHENG, C-1752, Rice University. MULTIPLE-DIMENSIONAL OPTICAL SPECTROSCOPY.

In last year, we made three major breakthroughs and one important measurement:

- (1) We demonstrated that three dimensional molecular conformations in condensed phases can be determined by measuring the cross angles among vibrational modes covering the entire molecular space by benchmarking the method with well defined crystalline samples. (*JPCA*, 117, 8407 and *JPCB*, 117, 15614).
- (2) We demonstrated that intermolecular distances smaller than nm in condensed phases can be determined by measuring intermolecular vibrational energy transfers by benchmarking the method with crystalline samples with known well-defined energy donor/acceptor distances. (*JPCA*, 118, 2463).
- (3) We experimentally and theoretically demonstrated that the experimentally observed nonresonant energy transfers in condensed phases are governed simultaneously by two mechanisms. The relative importance of these two mechanisms under different situations can result in some surprising

phenomena, e.g. inverted gap dependences of energy transfers, and opposite temperature dependences of resonant and nonresonant energy transfers. (*PCCP*. DOI: 10.1039/C4CP01300J).

(4) We developed a molecular rotational method that enables us to directly determine the solvent coordination number of Li cation in its solutions. (*JPCB*. 118, 3689).

HONGCAI JOE ZHOU, A-1725, Texas A&M University. EFFICIENT CARBON CAPTURE WITH FUNCTIONALIZED POROUS POLYMER NETWORKS (PPNs).

The current carbon capture and sequestration technology of removing CO₂ from flue gas streams of power plants, amine scrubbing, places an enormous parasitic power demand on the plant and thereby increases the cost of electricity.

We demonstrated that we can rationally build PPNS with multiple adsorption sites for binding CO₂ under ambient conditions. For example, PPN-6-SO₃NH₄ exhibits exceptionally high CO₂ capacity at low pressures and CO₂ over N₂ selectivity by using a variety of methods. Given its outstanding physicochemical stability and mild regeneration requirements, PPN-6-SO₃NH₄ has great potential for practical application in a post-combustion CO₂ capture technology.

We developed an easily accessible method to analyze data for carbon capture technologies. Any researcher can calculate working capacities per unit of regeneration energy at optimal desorption temperatures with a simple set of equations and procedures we have developed, given only the input of experimental data from adsorption isotherms and heat capacities of any material. The model also is useful in real settings as it provides a guide to which materials and what conditions that should be tested further.

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 2012-2013 Academic year. The group currently consists of fifteen 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 in 2013/2014. Dr. An's lab is well funded by grants from ETF, Johnson & Johnson, Merck, UT system Star awards, PanaMab, and the NIH. 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. Dr. An taught a drug discovery course during the 2013/2014 Spring semester at the UT Graduate School of Biomedical Sciences.

DANIEL W. ARMSTRONG, CHAIR Y-0026, The University of Texas at Arlington.

In a series of four papers we developed enantioselective separations for a variety of chiral molecules that had not been separated previously. This included a series of potential antimalarial compounds, the flinderoles and borreverines (which are natural products). A better understanding of the chiral recognition mechanisms of two different classes of chiral selectors was obtained through judicious use of principal component analysis and via thermodynamic studies respectively.

Using ionic liquids as "tools" we developed what is possibly the most effective and efficient analysis for water (and ethanol) in pharmaceutical ingredients and other liquid consumer products. A new barrier ionization discharge detector was evaluated and shown to be advantageous for water analysis (~100x more sensitive than conventional methods). Our newly developed approaches were shown to be far more sensitive, accurate and broadly applicable than conventional approaches.

Paired ion electrospray ionization mass spectrometry (PIESI-MS) was shown to be perhaps the most sensitive method known for detection of certain pesticides and herbicides. The mechanism of this sensitivity enhancement was investigated by utilizing a series of related symmetrical and unsymmetrical pairing agents and examining their behavior in ESI conditions. The enhanced sensitivity could be attributed to the surface activity of the unsymmetrical dications, which results in a concurrent strong partitioning of the anion to the aerosol droplet surface. Surface tension measurements of the anion/IPR complex were conducted, and a correlation between the observed ESI responses and the surface activity of the complex was found. The mechanism was further explored and explained based on the concepts of the equilibrium partitioning model (EPM).

M. ZOUHAIR ATASSI, CHAIR Q-0007, Baylor College of Medicine.

Botulinum neurotoxin type B (BoNT/B) initiates its toxicity by binding to synaptotagmin II (SytII) and gangliosides GD1a and GT1b on the neural membrane. We synthesized two 27-residue peptides that carry the BoNT/B binding sites on mouse SytII (mSytII 37-63) or human SytII (hSytII 34-60). BoNT/B bound to these peptides, but showed substantially higher binding to mSytII peptide than to hSytII peptide. The mSytII peptide inhibited almost completely BoNT/B binding to synaptosomes (snps) and displayed a high affinity. BoNT/B bound strongly to mSytII peptide and binding was inhibited by the peptide. Binding of BoNT/B to snps was also inhibited (~80 %) by a larger excess of gangliosides GD1a or GT1b. The mSytII peptide inhibited very strongly (at least 80 %) the toxin binding to snps, while the two gangliosides were much less efficient inhibitors requiring much larger excess to achieve similar inhibition levels. Furthermore, gangliosides GD1a or GT1b inhibited BoNT/B binding to mSytII peptide at a much larger excess than the inhibition by mSytII peptide. Conversely, BoNT/B bound well to each ganglioside and binding could be inhibited by the correlate ganglioside and much less efficiently by the

mSyII peptide. There was no apparent collaboration between mSyII peptide and either ganglioside. mSyII peptide displayed some protective activity *in vivo* in mice against a lethal BoNT/B dose. We concluded that SytII peptide and gangliosides bind independently but, with their binding sites on BoNT/B are spatially close, and each influences BoNT/B binding to the other by regional conformational perturbations or steric interference or both. Ganglioside involvement might help in toxin translocation and endocytosis. (*Protein J.* 2014 33(3):278-288).

In cervical dystonia, injection of botulinum neurotoxin (BoNT) A or B into affected neck muscle reduces symptoms but may elicit anti-toxin antibodies (Abs) that block responsiveness to treatment. Previously, we localized the BoNT/A and BoNT/B sites that bind mouse or human blocking Abs. We also reported that site-specific auto-Abs can be suppressed by a monomethoxypolyethylene glycol (mPEG)-epitope conjugate. So we elicited here anti-toxin Abs in outbred mice by immunization with sublethal-suboptimal doses of active BoNT/A and determined the efficacy of selected mPEG-epitopes in reducing established anti-BoNT/A Abs. We tested in outbred mice four synthetic mPEG-N(α)-epitopes [N8 (residues 547-565), N25 (785-803), C15 (1051-1069), C31 (1275-1296)] of BoNT/A in tolerance against ongoing anti-toxin Abs. After short immunizations, tolerization with an mPEG-peptide reduced Abs to correlate peptide and caused varying Ab reductions to the other three peptides. Anti-N8 Abs were unaffected by mPEG-N25 tolerization, but mPEG-N8 and mPEG-N25 caused drop in anti-BoNT/A Abs. After long immunization with BoNT/A, tolerization with mPEG-N8 lessened anti-N8 Abs. Anti-C15 Abs decreased by tolerization with mPEG-C15 or any other mPEG-peptide. Anti-N25 Abs were not altered by mPEG-N25, but decreased after tolerization with mPEG-C15. Anti-C31 Abs disappeared on day 474 by tolerization with mPEG-C31 or mPEG-N8, mPEG-N25 or mPEG-C15. When an Ab response returns, a decrease can be re-established by re-administering the correlate mPEG-peptide. The method may be beneficial for extending BoNT treatment in immunoresistant patients. (*J Neuroimmunol.* 2014 Jul 15;272(1-2):29-34.).

VYTAS A. BANKAITIS, CHAIR BE-0017, Texas A&M University Health Science Center.

We have made progress in four major areas this year.

Area 1—Sec14-like phosphatidylinositol transfer proteins (PITPs) integrate diverse territories of intracellular lipid metabolism with stimulated phosphatidylinositol-4-phosphate production, and are discriminating portals for interrogating phosphoinositide signaling. We validate the first small molecule inhibitors (SMIs) of the yeast PTP Sec14. These SMIs are *N*-nitrophenyl(4-(2-methoxyphenyl)piperazin-1-yl)methanones (NPPMs), and are effective inhibitors *in vitro* and *in vivo*. We further establish Sec14 is the sole essential NPPM target in yeast, that NPPMs exhibit exquisite targeting specificities for Sec14 (relative to related Sec14-like PITPs), propose a mechanism for how NPPMs exert their inhibitory effects, and demonstrate NPPMs exhibit exquisite pathway selectivity in inhibiting phosphoinositide signaling in cells. These data deliver proof-of-concept that PTP-directed SMIs offer new and generally applicable avenues for intervening with phosphoinositide signaling pathways with selectivities superior to those afforded by contemporary lipid kinase-directed strategies. This work was published as cover article in the January 2014 issue of *Nature Chemical Biology*.

We also collaborated with the Giaever lab to complete a comprehensive chemogenomic analysis of the druggable proteome of budding yeast. This effort involved a large-scale chemogenomic screen of 15 million drug-gene interactions and provided a systems-level view of the cellular response to small molecule perturbation. Unexpectedly, we found the cellular response to drug is restricted, and can be captured by as few as 45 gene signatures. The data are also translatable as structural chemical properties predict which molecules may cause drug-induced phospholipidosis, a phospholipid storage disorder, in humans. Moreover, we described a resource of 317 chemical-genetic probes for inhibition of a set of 121 genes. This work was published as a highlighted article in the April 15, 2014 issue of *Science*.

We have also generated a series of reagents where we can purify a group of fascinating lipid binding proteins that control lipid signaling and analyze their various binding ligands and mechanisms of function as molecules. Crystallography is part of the plan as is subjecting these proteins to sophisticated biophysical analyses to understand the conformational transitions required for their function.

Area 2—Lipid droplet (LD) utilization is an important cellular activity that regulates energy balance and lipolytic release of lipid second messengers. As fatty acids exhibit both beneficial and toxic properties, their release from LDs must be controlled. Herein, we demonstrate yeast Sfh3, an unusual Sec14-like phosphatidylinositol transfer protein (PITP), is an LD-associated protein that inhibits lipid mobilization from these particles. We further document a complex biochemical diversification of LDs during meiosis wherein Sfh3, and select other LD proteins, redistribute into discrete LD subpopulations. The data report Sfh3 modulates the efficiency with which a neutral lipid hydrolase-rich LD subclass is consumed during biogenesis of specialized membrane envelopes which package the haploid meiotic genomes. These results present novel insights into the interface between phosphoinositide signaling and developmental regulation of LD metabolism, and unveil meiosis-specific aspects of Sfh3 (and phosphoinositide) biology that are invisible to contemporary haploid-centric cell biological, proteomic and functional genomics approaches. This work was published as cover article in the March 1 2014 issue of *Molecular Biology of the Cell*.

Area 3—Root hairs are elongated extensions of plasma membrane designed for efficient nutrient absorption. Their development involves a polarized membrane growth program which initiates at a precise position on the root hair epidermal cell plasma membrane. The *Arabidopsis* AtSfh1 protein is critical for root hair biogenesis, and it is comprised of an N-terminal Sec 14-domain and a C-terminal nodulin domain of the Nlj16 family. We now show how the unique modular domain organization of AtSfh1 regulates phosphatidylinositol-4,5-bisphosphate [PtdIns(4,5)P₂] signaling in polarized root hair growth. The Sec 14-domain supports phosphatidylinositol-4,5-bisphosphate [PtdIns(4,5)P₂] synthesis, and PtdIns(4,5)P₂ subsequently directs multiple aspects of the root hair tip-growth program. We demonstrate that the AtSfh1 nodulin domain is a high-affinity PtdIns(4,5)P₂ binding module, and that AtSfh1 PtdIns(4,5)P₂-binding activity is required for polarized PtdIns(4,5)P₂ distribution during root hair development. These data describe how AtSfh1 employs its two domains cooperatively to pattern PtdIns(4,5)P₂ microdomains for coherent phosphoinositide signaling during active tip-growth. Interestingly, we find the lateral

sequestration activity of these lipid-binding domains to be tunable so that signaling can occur with exquisite spatial and temporal resolution. These discoveries suggest a biological rationale for why legumes produce Nlj16-like nodulins during nodulogenesis. This Ghosh et al manuscript is now in revision.

Area 4--We described a new set of protein:protein interactions involving the cystic fibrosis transmembrane regulator (CFTR) protein that govern its trafficking itinerary through the mammalian endomembrane system. The insights gained suggest new ideas for manipulating the system to reduce the severity of cystic fibrosis. This McDermott et al manuscript is now in revision after a round of positive reviews.

ALLEN J. BARD, CHAIR F-0021, The University of Texas at Austin.

Over the reporting period we have developed a new emulsion characterizing method by single droplet collision. We have also suggested two methods to observe single collision events of single emulsion droplets.

- Emulsion droplet reactor (EDR): observing electrochemical oxidation of ferrocene in toluene emulsion droplets.

-Emulsion droplet blocking (EDB): observing the blocking effect of ferrocyanide in continuous phase by toluene emulsion droplet collision.

We are also nearing completion of studies of selective reduction of nitrobenzene droplets and 7,7,8,8-tetracyanoquinodi methane in nitrobenzene droplets.

We also continue using SECM-based combinatorial methods to screen photocatalysts and investigate their photoelectrochemical (PEC) properties.

ANDREW R. BARRON, CHAIR C-0002, Rice University.

Amine-based absorbents play a central role in the development of CO₂ sequestration and utilization technologies. Amines react selectively with CO₂, and high CO₂ absorption capacities are obtainable when the amine portion of the absorbent is maximized. Based on these premises, amine-rich compounds can be converted to high capacity and highly selective CO₂ absorbents using proper cross-linkers. Polyethyleneimine (PEI) conjugates with a range of nanocarbons (NCs) have been prepared, and their performance with regard to carbon dioxide absorption and liberation are compared. PEI-functionalized MWNTs prepared by the reaction of branched PEI with F-MWNTs showed a lower CO₂ capacity at 25 °C (5 wt%) as compared to PEI-SWNTs (9.2 wt%) consistent with the interior layers of the MWNTs adding weight to the base NC without adding functionality. PEI-functionalized graphite/graphene was prepared and the CO₂ capacity of PEI-GO at 25 °C (8 wt%) was comparable to that of PEI-SWNTs making GO a valid and cheaper alternative to the SWNT scaffold. The temperature of CO₂ desorption of the PEI-NCs was 75 °C providing a lower energy load for regeneration compared to current amine-based scrubbing units. The rate of CO₂ uptake is seen to depend on the curvature of the NC substrate. Based upon these results we have developed a new concept where an amine-rich compound, PEI is converted to a high capacity and highly selective CO₂ absorbent using C₆₀ as a cross-linker. The CO₂ absorption performance of the resulting hybrid, PEI-C₆₀, is compared to that of one of the best classes of gas absorbents available to date, metal organic frameworks (MOFs), to show that PEI-C₆₀ can perform better than metal-organic-framework compounds (MOFs) in critical applications like the abatement of CO₂ in the sweetening of natural gas.

RAY H. BAUGHMAN, CHAIR AT-0029, The University of Texas at Dallas.

Welch Chair support helped enable seven publications during the report period, including one publication in *Science* and two in *Nature Communications*. In the *Science* publication we demonstrated that inexpensive high-strength polymer fibers used for fishing line and sewing thread can be easily transformed by twist insertion to provide fast, scalable, nonhysteretic, long-life tensile and torsional muscles. Extreme twisting produces coiled muscles that can contract by 49%, lift loads over 100 times heavier than can human muscle of the same length and weight, and generate 5.3 kilowatts of mechanical work per kilogram of muscle weight. In our two publications in *Nature Communications*, we demonstrated woven carbon-nanotube-based biofuel cell textiles that deliver high areal power densities while operated in human serum and torsional carbon-nanotube-based artificial muscles that use a spider-derived biomimetic strategy to combine up to 9,800 r.p.m. rotation speeds with oscillation-free angular controllability. In our other supported publications we described (1) supercapacitor textiles of MnO₂-containing, twist-spun carbon nanotube (CNT) yarns that provide high energy storage and power densities, (2) all-solid-state carbon nanotube torsional and tensile electrochemical muscles that provide giant torsional strokes and can lift heavy loads, (3) the fabrication and characterization of novel peptide/CNT composites, and (4) highly electronically conducting yarns in which CNTs are "biscrolled" as a guest in an electrospun polymer nanofiber host. The Welch Chair supported NanoExplorer high school students (36 strong in the program year), as well as past NanoExplorers, who have continued to make breakthroughs at UT Dallas. The Welch Chair and NISE Network in partnership with the Perot Museum of Nature and Science funded our participation in NanoDays 2014. Welch Chair seed funding was leveraged to obtain NanoTech Institute funding from the United States Air Force, the United States Navy, NASA, the US Korea NBIT III program, and numerous companies.

TADHG P. BEGLEY, CHAIR A-0034, Texas A&M University.

Molybdopterin biosynthesis: The enzyme MoaA catalyzes the first step in molybdopterin biosynthesis. This reaction involves the insertion of C8 of the purine into the C2'-C3' bond of the ribose. We have now completed a mechanistic characterization of this reaction. Our strategy involved trapping of the radical at C3', trapping of the addition product of this radical to C8 of the purine and exploration of the later steps in the reaction using 2'-deoxyGTP.

Riboflavin catabolism: We have now identified a riboflavin catabolic operon in a bacterial strain that we isolated from the DSM riboflavin production plant in Switzerland. We have overexpressed each of the proteins and identified a riboflavin lyase as the first step in the pathway. Mechanistic studies on this enzyme are in progress.

Menaquinone biosynthesis by the futasoline pathway: Our studies have focused on characterizing the mechanism of MqnE. This enzyme catalyzes the addition of the adenosyl radical to dehydrated chorismate followed by rearrangement. We have successfully reconstituted the reaction and characterized the mechanism using substrate analogs (Manuscript in preparation).

Heme catabolism: While heme is ubiquitous in the environment, we had a difficult time isolating heme catabolic bacteria. In the end, screening of a soil sample obtained from a temple in Nepal, where animals have been regularly sacrificed over several hundred years, yielded the needed catabolic strains. We have now cloned and sequenced the catabolic operon and are just beginning biochemical studies.

WESTON T. BORDEN, CHAIR B-0027, University of North Texas.

During the past year, one subject of my group's research has continued to be the use of negative ion photoelectron spectroscopy (NIPES) to measure singlet-triplet energy differences. In collaboration with Dr. Xue-Bin Wang at PNNL we showed: (a) Unlike $(\text{CO})_4$, $(\text{CS})_4$ has a singlet ground state, as we had predicted would be the case. (b) *meta*-Benzoquinone has a triplet ground state, and the relative energies of the two lowest singlet states are as we had calculated. (c) A D_{3h} geometry is a mountain top on the potential energy surface for singlet $(\text{CO})_3$, and the C_{2v} geometry of the triplet that can be accessed by NIPES from $(\text{CO})_3$ is a transition structure on the triplet potential energy surface. Our theoretical and experimental studies of $(\text{CO})_4$ led us to carry out calculations on $(\text{SiO})_4$; and, as we expected would be the case, the triplet is predicted to be lower in energy than the singlet at the lowest energy D_{4h} geometry of each state. However, unlike the case in $(\text{CO})_4$, the lowest singlet state of $(\text{SiO})_4$ is predicted to have a strong preference for a tetrahedral, rather than a square planar geometry. We were able to explain why the geometries of singlet $(\text{CO})_4$ and singlet $(\text{SiO})_4$ should differ. In collaboration with Professor Ronald Hoffmann, we showed how to design a carbene with a $\sigma^0\pi^2$ singlet ground state, and we also predicted that tunneling would change the preferred product formed by rearrangement of noradamantylmethyl carbene from ring expansion at high temperatures to hydrogen migration at cryogenic temperatures. Finally, in collaboration with Professor Wolfram Sander, we investigate the role of tunneling in the ring opening of a highly strained cyclopropene to a carbene.

ALAN H. COWLEY, CHAIR F-0003, The University of Texas at Austin.

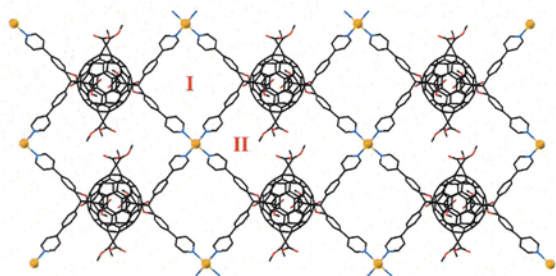
The research effort over the past year has been focused on five general areas. The first area of research was focused on the functionalization of the bis(imino)acenaphthene (BIAN) ligand class. The pathways for achieving BIAN functionalization have been identified and used for the development of an array of new redox-active ligands. The second area of research was concerned with the application of BIAN based N-heterocyclic carbene ligands for use in palladium catalyzed carbon-carbon (Suzuki-Miyaura) coupling reactions. The foregoing complexes were used in both a homogeneous and a heterogeneous fashion. Thirdly, the acenaphthene motif was investigated for use as a ligand support for cobalt macrocycles (cobaloximes) that are very useful for small molecule transformations. Molecules of this type have been stabilized with respect to chemical reduction, thus allowing for greater insight into the mechanistic intermediates that are involved in cobalt small molecule catalysis. A fourth aspect of the current research involved investigation of solid state BIAN photoluminescence. Recently, it has been demonstrated that zinc coordination complexes of the BIAN ligand emit tunable solid state photoluminescent emissions. The nature and control of these emissive complexes is currently under investigation. Finally, novel sterically shielded N-heterocyclic carbene palladium complexes have been developed as highly efficient catalysts for chloroarene hydrodechlorination.

RICHARD M. CROOKS, CHAIR F-0032, The University of Texas at Austin.

We have been interested in learning how the physical and chemical properties of catalysts affect their selectivity and efficiency. Nanoscale catalysts in the 1-3 nm size range are of particular interest, because very slight changes to materials in this size range can dramatically affect their catalytic properties. Accordingly, our group uses a versatile, template-based method, discovered by our group, to synthesize metal nanoparticles that have remarkable uniformity in size, composition, and structure. One important lesson we have learned during the course of these studies is that there are not many good analytical methods for studying the characteristics and properties of nanoparticles smaller than about 3 nm, and therefore we also invented and modified analytical methods to suit our needs. Our nanoparticle catalysis work is guided by theoretical calculations thanks to a long-standing collaboration with the Henkelman group here at UT. The Crooks group also has a long-standing interest in chemical and biological sensors. Over the past two to three years we have directed this activity toward the development of ultra-low cost sensors (<\$1), primarily for medical applications in both the developed and developing world. In most cases these sensors are constructed of paper, fabricated by origami, and the result of the assay detected using electrochemical methods. New principles and analytical methods are required to keep the cost of these devices low and the detection limits appropriate for a particular application. Finally, we have developed a new electrochemical method for desalinating salt water that is highly energy efficient. We have a basic understanding of the phenomena responsible for its effectiveness but are still studying the fundamental principles of the method. At the same time we are working with a small company to commercialize the desalination technology.

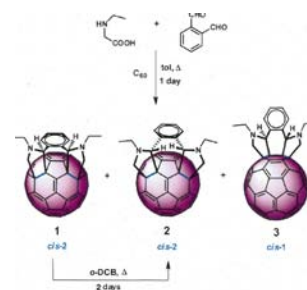
LUIS ECHEGOYEN, CHAIR AH-0033, The University of Texas at El Paso.

This report covers the progress made since July, 2013. Welch Foundation support was acknowledged in twenty-two publications in last year's report and this year we acknowledge fourteen new articles, ranging in research topic from Dye Sensitized Solar Cells (DSSCs) to empty and endohedral fullerene

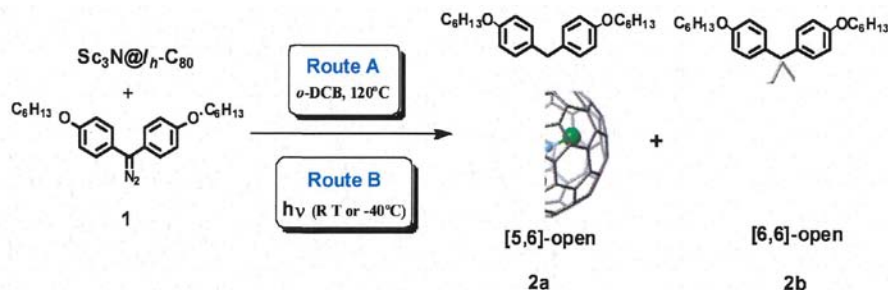


derivatives and Metal Organic Frameworks (MOFs). Three of these articles were published in *Angew. Chem. Int. Ed. Eng.*. In one article we reported the first example of a fullerene-linker based 2D MOF, using pyridyl ligands and Cd^{2+} , see X-Ray crystal structure. We are currently actively pursuing the synthesis of a 3D version of a fullerene-linked based MOF, which should possess large and rigid pores and exhibit high hydrogen absorbing capabilities. In a related development we prepared a new benzothiazole-linked nanoporous polymer which exhibits a reasonable CO_2 adsorption capacity (7.8 wt%) with good selectivities, $\text{CO}_2/\text{N}_2 = 51$ and $\text{CO}_2/\text{CH}_4 = 6.3$.

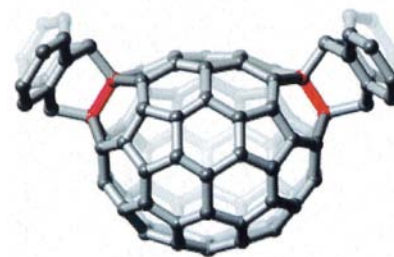
We continued to make significant progress in our fullerene work, introducing new reagents for tethered b/s-functionalization on empty fullerenes, see structures. The two *cis*-2 *bis*-pyrrolidine adducts of C_{60} exhibit an unprecedented diastereomeric relationship and, while structurally being very similar, they possess very different physical and chemical properties. A *cis*-1 tethered *bis*-adduct was also isolated chromatographically, see structure. We were also able to isolate and characterize the first example of a [5,6] open methano-adduct of an endohedral fullerene, which also possesses unique properties, especially electronically, see structure **2a**. This finding opens new avenues for novel endohedral fullerene derivatives with unusual electronic properties and potential applications in photovoltaic devices. We are exploring similar diphenylmethane additions with varying chain lengths in order to control solubility and film deposition. In addition to working with the Sc-based endohedral we are also working with the analogous Y and Lu trimetallic nitrides. An overview of the size, shape and electronic complementarity between the carbon cages and the encapsulated clusters of endohedral fullerenes was also published with Welch acknowledgement.



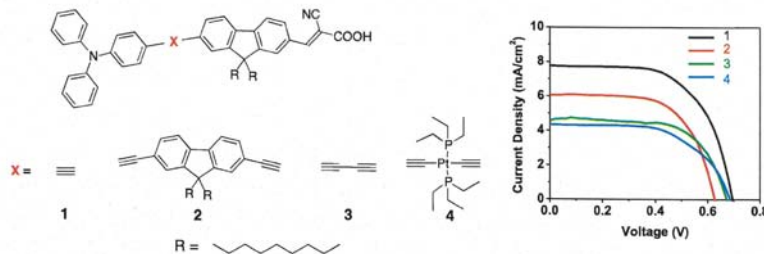
Considerable progress was also made in the Carbon Nano-Onion (CNO) area. We have been mainly concerned with the applications of CNO derivatives as materials for supercapacitor electrodes and as selective sensors. A critical review acknowledging Welch support was published in *J Mat Chem. A*.



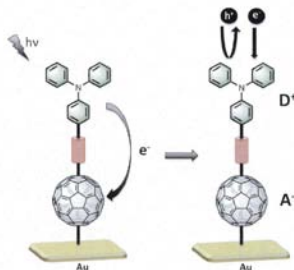
On another fullerene multi-adduct project, we found that the reaction between melted anthracene and C_{70} leads to a remarkably regioselective *bis*-adduct, a very similar observation to what was reported in 1996 by Kräutler between melted anthracene and C_{60} . When two equivalents of melted anthracene and solid C_{70} are heated under vacuum, only two products are obtained, a Diels-Alder *mono*-adduct on one of the a bonds and a single *bis*-adduct, where the two anthracenes are disposed exclusively in the so-called 12-o'clock configuration, with no evidence of any additional isomeric *bis*-adducts, see X-Ray structure. This highly regioselective reaction yields 68% of the unique *bis*-adduct, so it is currently being evaluated in solar cells, but the thermal retro-Diels-Alder reaction is making cell fabrication a serious challenge.



On a final summary note, we made substantial progress which resulted in two published articles in the field of DSSCs, after successfully designing and synthesizing several new organic dyes, mainly containing triphenylamine donor groups. A variety of different types of linkers and TiO₂ anchoring groups were tested to probe the relative importance of HOMO-LUMO delocalization in the ground and excited states of the dyes and for effective attachment and charge injection into the TiO₂ electrodes, see some of the structures above. Photoconversion efficiencies up to 3.8% were obtained for the best cases.



Finally, we also published an article showing that donor-acceptor (DA) dyad self-assembled -monolayers (SAMs) can effectively act as photoswitched interfacial layers to selectively extract electrons from solution. The idea is that upon photoexcitation the TPA donates an electron to the fullerene, thus creating an intramolecular charge separated state, which generates positive charge on the SAM surface and is capable of rejected holes and attracting electrons. This work was mainly performed using electrochemical impedance spectroscopy. This proof of concept (see schematic diagram) opens the way for other systems that could act as photoswitches for the selective hole as well as for electron extraction from photoactive layers in solar cells.



J. RUSSELL FALCK, CHAIR I-0011, The University of Texas Southwestern Medical Center.

Contributions to synthetic methodology include: (1) an exceptionally mild, direct N-H and N-alkyl aziridination of olefins via Rh-catalysis; (2) instance of intramolecular cyanation of a styrene by a rhodium-catalyzed N-CN cleavage reaction; and (3) a review of selective C-C/O-C/N-C activation by transition metals. In a series of collaborative studies, we reported; (1) the protective mechanisms of 5,14-HEDGE, a 20-hydroxyeicosatetraenoic acid (20-HETE) mimetic, against the symptoms of septic shock; (2) results suggesting 20-HETE mediates androgen-induced hypertension as well as cause hypertension independent of androgen; (3) cytochrome P450 2J2 overexpression protects against arrhythmia susceptibility in cardiac hypertrophy; 20-HETE regulates the angiogenic functions of human endothelial progenitor cells and contributes to anmgiogenesis *in vivo*; (4) 20-HETE induces remodeling of renal resistance arteries independent of pressure elevation in hypertension; (5) increases in 20-HETE associated with a decreased production of prostanoids and nitric oxide contribute to the ability of NS-398 to prevent hypotension during septic shock; (6) orally active epoxyeicosatrienoic acid (EET) analogs attenuate kidney injury in hypertensive Dahl salt-sensitive rats; (7) EET analogs promote organ and tissue regeneration; (8) EET analogs attenuate cisplatin nephrotoxicity; (9) EETs protect cardiac cells during starvation by modulating an autophagic response; (10) acyl-homoserine lactone synthase YenI from *Yersinia enterocolitica* modulates virulence gene expression in Enterohemorrhagic *E. coli* O157:H7 and (11) the 15-lipoxygenase metabolites erythro-13-hydroxy-14,15-epoxyeicosatrienoic acid and 11(R),12(S),15(S)-trihydroxyeicosatrienoic acid significantly relaxed mouse mesenteric arteries.

ANDREW FUTREAL, CHAIR G-0040, The University of Texas M.D. Anderson Cancer Center.

We have made substantial progress over the last year. The Welch funds have been instrumental in moving rapidly on several projects – all focused on the study of genetic heterogeneity and tumor phenotype. First, we have been pursuing work in the rare tumor type Sarcoma. In particular, studying angiosarcoma, a rare tumor of blood vessel origin. We have worked on the identification of recurrent mutations in two genes that sit along a key pathway that regulates blood vessel cell growth (angiogenesis). This pathway is already a key area of focus for therapeutics and these findings bring a new genetic focus to this work, including an opportunity to understand responder and non-responder biology. This work has been recently published in *Nature Genetics*. Further, we are currently more fully exploring this discovery in a larger panel of patient samples in a comprehensive look at the entire signaling circuitry involved in angiogenesis pathways and response to therapy. This work was also the subject of a platform presentation at the prestigious ASCO (American Society of Clinical Oncology) meeting earlier this year. More recently, again utilizing the Welch funds to move rapidly and strategically, we have completed a study that,

for the first time, elucidates the heterogeneity within individual patient's lung cancers. This is our first look at the spatial and temporal genomic architecture and complexity of the most common cancer. We focused our work on localized disease (no distant metastasis) and found that there is substantial regional difference in mutations from one part of the tumor to another. Strikingly, 21/22 mutations in known cancer genes are present throughout all parts of the tumor. This is in stark contrast to our prior work on kidney cancer. Further, and perhaps most interestingly, whilst we were working on this contemporary cohort of patient samples, three patients suffered relapses. We then analyzed the data and found that there is a statistically significant association of increased complexity of the tumor and risk of relapse. We are moving rapidly to a much larger confirmation study. If this result holds, it could be practice changing for early stage lung cancer – suggesting that some early stage lung cancers may benefit from adjuvant therapy in what is a heretofore-surgical setting. This work has been accepted for publication in *Science*.

JAN-ÅKE GUSTAFSSON, CHAIR E-0004, University of Houston.

This year we have focused on the roles of ER β and LXR β in: (1) mouse models of multiple sclerosis and Parkinson's disease; [2] breast and prostate cancer; (3) glucose and lipid homeostasis. We have obtained crystals of the LXR β -RXR DBD-LBD dimer complex with DNA and solved the crystal structure. This work has provided new insights into how these receptors are able to distinguish among different DR4 elements on DNA. We discovered two ER β -regulated genes (DACH1 and Foxo3A), induced by ER β -selective agonists that are important in repressing proliferation of breast and prostate tissue. We have also found that ER β -selective ligands repress microglial activation in mouse models of ALS and MS. Thus ER β agonists continue to be promising novel pharmaceuticals in the treatment of prostate cancer and neurodegenerative diseases. We have used spinal cord samples to localize ER β and LXR β in human spinal cords. The distribution of these receptors in human spinal cords is similar to that in mice. In addition, ER β represses proliferation in human microglial cells in culture. These results give us confidence that the mouse models will provide information relevant to human diseases.

WILLIAM L. HASE, CHAIR D-0005, Texas Tech University.

Progress was made in the development of models, algorithms, and computer programs for chemical dynamics simulations, and in the application of this software to research problems of significant chemical interest. The Hase research group continues to develop the VENUS computer program for performing chemical dynamics simulations and significant progress was made in maintaining a web-based portal for this software, which will make it very accessible and easy to use by other research groups and scientists. The portal includes a repository of all the models the Hase research group has used for their simulations. The Hase research group also develops, maintains, and distributes the VENUS/NWChem software package for direct dynamics simulations. The specific research problems reported here are: 1) effect of microsolvation on chemical reaction dynamics; 2) dynamics of gas-phase S_N2 reactions; 3) interaction of chemical warfare agents with oxide surfaces; 4) collisions of rare gas atoms with ice surfaces; 5) photophysics of solar cells; 6) development of algorithms and software for chemical dynamics simulations (including direct dynamics); 7) theory of unimolecular and intramolecular reaction dynamics; 8) intermolecular potentials and dynamics for collisions of projectile ions with organic surfaces; 9) hypersonic ignition of bipropellants; and 10) intermolecular energy transfer in the liquid and gas phases.

ALLAN J. JACOBSON, CHAIR E-0024, University of Houston.

Synthesis and Characterization of Novel Metal Oxides: The synthesis and characterization of new transition-metal oxide organic compounds is investigated. We have investigated reactions of both lanthanide hydrated metal nitrates and lanthanide oxides directly with formamide have been studied. Fifteen lanthanide formate frameworks were obtained under mild solvothermal reactions, nine were isostructural compounds with the composition Ln(HCOO)₃·(HCONH₂)₂ and six were isostructural anionic frameworks [CH(NH₂)₂][Ln(HCOO)₄]. All compounds contain metal ions eight coordinated by oxygen atoms connected by *anti-anti* formate ligands to form frameworks. The reaction chemistry demonstrated for simple may be applicable for acid free, environmental-friendly rare earth metal recovery from a variety of end-of-use products. We have also investigated redox intercalation into the host lattice, vanadium benzenedicarboxylate, VOBDC with the electroactive guest molecule hydroquinone.

Solid State Ionics: The structure and properties of mixed conducting oxides in thin film and bulk form are investigated. In recent work, neutron powder diffraction was used to characterize the layered perovskites PrBaCO₂O₅ + and NdBaCo₂O_{5+ δ} under *in-situ* conditions from 573 to 852 °C and at pO₂ = 10⁻¹–10⁻⁴ atm. The oxygen vacancies were found to be localized within the Pr or Nd layers. The location of these vacancies and the anisotropic displacement of the surrounding oxygen anion sites indicate that ion transport occurs via a hopping mechanism between O sites in the Pr layer and the nearest neighbor sites in the Co layer. In a related project, chemical oxygen diffusion coefficients and chemical surface exchange rates along with oxygen self-diffusion coefficients in dense samples of Sr₃YCO₄O_{10.5+ δ} were studied by using a combination of electrical conductivity relaxation measurements and thermogravimetric analysis data in the temperature range of 650 °C – 900 °C. The results are in excellent agreement with previous studies using isotope exchange and depth profiling.

WILLIAM H. KLEIN, CHAIR G-0010, The University of Texas M. D. Anderson Cancer Center.

This past year, we completed our analysis of the transcriptome of Atoh7-expressing cells in embryonic retinas. Atoh7 is a transcription factor necessary but not sufficient for the initial specification of ROCs. Using FACS purified GFP-labeled Atoh7-expressing retinal progenitor cells (RPCs), we performed RNA-seq and generated a dataset containing genes that were enriched and de-enriched in Atoh7-expressing RPCs. From the analysis we identified 1,497 transcripts that were significantly enriched or de-enriched. We chose to focus primarily on transcription factors enriched in Atoh7-RPCs and found that two in particular merited further attention. One was an ortholog of the Drosophila eyes absent gene called Eya2 and the other a factor called Ebf3. We recently published a report describing these results and demonstrating that both Eya2 and Ebf3 are direct target genes of Atoh7. We also showed that Eya2 is

genetically positioned downstream of *Atoh7* and upstream of *Pou4f2*, a transcription factor required for the normal differentiation of RGCs. In contrast, *Ebf3* is downstream of *Pou4f2*. Our findings led to a new regulatory pathway for RGC development: *Atoh7* \Rightarrow *Eya2* \Rightarrow *Pou4f2* \Rightarrow *Ebf3*. We hypothesized that *Eya2* is involved in the early specification event and that *Atoh7* and *Eya2* work together to activate the genes required for RGC specification. Notably, *Eya2* is a dual function protein that is an atypical protein phosphatase as well as an activator of gene expression. To test our hypothesis we have constructed a series of *Eya2* vectors and are in the process of generating mice containing the *Eya2*-modified alleles. Namely, two separate vectors for producing *Eya2*-null alleles, a *Rosa-Stop-lack-Eya2* vector for over expressing *Eya2* and an *Eya2-Delta* phosphatase domain vector for determining whether the role of protein dephosphorylation by *Eya2* in the developing retina. In the next period, we plan to analyze the retinas of these genetically engineered mice.

MICHAEL J. KRISCHE, CHAIR F-0038, The University of Texas at Austin.

The formation of C-C bonds is fundamental to the endeavor of chemical synthesis. The largest volume application of homogenous metal catalysis is alkene hydroformylation, which may be viewed as the prototypical C-C bond forming hydrogenation. Our laboratory is engaged in the first systematic efforts to develop C-C bond forming hydrogenations beyond hydroformylation; processes wherein two or more reactants are hydrogenated to form a single, more complex product. Using cationic rhodium and iridium catalysts, we have found that diverse π -unsaturated reactants reductively couple to carbonyl compounds and imines under hydrogenation conditions, offering a byproduct-free alternative to stoichiometric organometallics in a range of classical C=X (X = O, NR) addition processes. This concept is extended further via "*C-C bond forming transfer hydrogenation*"; processes wherein hydrogen exchange between alcohols and unsaturated reactants serves to generate aldehyde-organometal pairs that combine to give products of carbonyl addition or hydrohydroxyalkylation. Direct alcohol CH-functionalization in this manner is again byproduct-free, and avoids discrete redox manipulations often required to convert alcohols to aldehydes.

Several major advances were made in the 2013-2014 funding period. In the presence of simple ruthenium(0) catalysts, cyclic diols and acrylic esters, which are abundant commodity chemicals, engage in C-C coupling to form spirolactones [*J. Am. Chem. Soc.* 135, 17230-17235 (2013)]. It was found that α -olefins, which are direct products of petroleum cracking and, hence, are vastly abundant, will engage in C-C coupling with certain vicinally deoxygenated reactants upon exposure to ruthenium(0) catalysts [*Angew. Chem. Int. Ed.* 52, 8428-8431 (2013)]. The ability to directly functionalize alcohol C-H bonds continues to avail new streamlined, strategies for the synthesis of natural products, as illustrated in the total synthesis of the anti-cancer compounds (+)-trienomycins A and F [*J. Am. Chem. Soc.* 135, 1098610989 (2013)], which were prepared in half the steps previously required. Indeed, our program in natural product total synthesis has flourished to the point that we were invited to review our collective studies on the synthesis of type I polyketides via alcohol C-H functionalization [*Nat Prod. Rep.* 31, 504-513 (2014)].

JAMES C. LEE, CHAIR H-0013, The University of Texas Medical Branch at Galveston.

In the project to elucidate the mechanism for the evasion of antibody neutralization in viruses we have successfully developed a quantitative mechanism to link flexibility of epitopes to affinity to antibody binding and to link long-range communication between distant residues to the epitopes and the effects of such linkage on the binding affinity of antibody; established a *quantitative* correlation between the magnitude of energetic susceptibility of the epitope (quantified as energy of coupling) and the decrease in MAb binding affinity. Thus, the current dogma that an epitope is located in a flexible region is *only a required but not sufficient* parameter in the binding to antibodies *per se*.

Bone morphogenetic proteins (BMPs), consisting of about twenty members, are members of the transforming growth factor- β (TGF- β) superfamily. BMPs show diverse functions but with limited number of receptors. Thus, a challenge is to understand the mechanisms of macromolecular recognition and specificity. The present study shows that different residues located in the ligand-receptor contact sites play different role in defining ligand affinity. Protein dynamics plays a significant role in defining affinity (maybe specificity) in BMP-receptor interactions in addition to specific residue interactions. Computation analysis using COREX/BEST and Molecular Dynamics simulation reveal that the overall patterns of long distance communication within the two forms of BMPR-1A and -1B are similar, although there is larger effect in perturbing the network of connectivity by natural disease-causing mutants for BMPR-1B than BMPR-1A and the quantitative values are different. Thus, these results imply that the fold of the protein and the sequence in combination affect the long-range interactions in BMPR-1 ECD.

PHILIP D. MAGNUS, CHAIR F-0018, The University of Texas at Austin.

During the budget period, three students whose research program was supported either partially or fully by the R. P. Doherty, Jr.-Welch Chair in Chemistry received their master's degrees. Two of those students have continued in the doctoral program although with different supervisors following the retirement of Professor Magnus. During the budget period, one student received his PhD.

BETTIE SUE MASTERS, CHAIR AQ-0012, The University of Texas Health Science Center at San Antonio.

We recently published our mouse model studies, which produced a conditional knockout (CKO) of POR in bone by crossing *Por* (*lox/lox*) and *Dermo1 Cre* mice, but did not affect liver reductase, showing the specificity of the knockout. Human patients, with specific POR mutations, exhibit severe developmental malformations, including disordered steroidogenesis, sexual ambiguities and various bone defects. CKO mice were smaller than littermate controls and exhibited significant craniofacial and long bone abnormalities. The deleterious effects of conditional deletion of POR from bone on both skull development and long bone trabecular density, as measured by micro computed tomography, were shown. Bone-specific deletion of POR affected fibroblast growth factor receptor-mediated signaling, with downregulation of *Runx2*, *Sp7* and upregulation of *Sprouty*—critical for bone development—in long bone, suggesting that the POR/CYP system is involved. Many CYP metabolites are involved in bone development, but the presence and roles of CYPs in bone are

not well-studied. We demonstrated CYP1A2 (aryl hydrocarbons), CYP2E1 (acetaminophen), CYP19 (testosterone), CYP17A1 (progesterone), CYP26A1 (retinoic acid) and weaker 2R1 (vitamin D) expression in the growth plate of mouse long bones and decreased expression of all CYPs in the mouse bone-specific POR deletion.

DAVID D. MOORE, CHAIR Q-0022, Baylor College of Medicine.

We are characterizing the roles of nuclear receptor ligands in diverse disease models. A primary focus this year has been on the roles of nuclear receptors in cell stress pathways. The first of two related projects focused on the nuclear receptor LRH-1 and its role in cell stress, particularly endoplasmic reticulum (ER) stress. We have found that mice lacking LRH-1 in the liver show increased sensitivity to tunicamycin, a standard inducer of ER stress. These mice are fully able to activate the evolutionarily conserved survival pathway induced by ER stress, termed the unfolded protein response (UPR), but are unable to complete the response and restore normal cell function. We found that this is due to loss of a new pathway for resolution of ER stress in which LRH-1 induces the kinase PIK3, which in turn phosphorylates the transcription factor Atf2. Activation of LRH-1 with a synthetic ligand improves the ability of hepatocytes to resist ER stress. Thus, our discovery of this new stress response provides a novel means to pharmacologically manipulate the ER stress response.

When a cell is starved, it breaks down its own proteins and other components to "recycle" nutrients, a process that is termed autophagy. Autophagy is induced in the fasted liver and repressed in the fed liver, and we have recently studied the role of nuclear receptors as regulators of this process. The nuclear bile acid receptor FXR and the nuclear fatty acid receptor PPARalpha are activated in the fed and fasted states, respectively. We have found that an FXR synthetic agonist can shut off autophagy in the fasted liver, while a synthetic PPARalpha agonist can induce it in the fed state. This provides a novel chemotherapeutic approach to modulation of this key cellular process.

ERIC N. OLSON, CHAIR I-0025, The University of Texas Southwestern Medical Center.

The adult mammalian heart has limited potential for regeneration. Thus, after injury, cardiomyocytes are permanently lost, and contractility is diminished. In contrast, the neonatal heart can regenerate owing to sustained cardiomyocyte proliferation. Identification of critical regulators of cardiomyocyte proliferation and quiescence represents an important step toward potential regenerative therapies. Yes-associated protein (Yap), a transcriptional cofactor in the Hippo signaling pathway, promotes proliferation of embryonic cardiomyocytes by activating the insulin-like growth factor and Wnt signaling pathways. We reported that mice bearing mutant alleles of Yap and its paralog WW domain containing transcription regulator 1 (Taz) exhibit gene dosage-dependent cardiac phenotypes, suggesting redundant roles of these Hippo pathway effectors in establishing proper myocyte number and maintaining cardiac function. Cardiac-specific deletion of Yap impedes neonatal heart regeneration, resulting in a default fibrotic response. Conversely, forced expression of a constitutively active form of Yap in the adult heart stimulates cardiac regeneration and improves contractility after myocardial infarction. The regenerative activity of Yap is correlated with its activation of embryonic and proliferative gene programs in cardiomyocytes. These findings identify Yap as an important regulator of cardiac regeneration and provide an experimental entry point to enhance this process.

Myocardium-related transcription factors (MRTFs) regulate cellular contractility and motility by associating with serum response factor (SAF) and activating genes involved in cytoskeletal dynamics. We reported previously that MRTF-A contributes to pathological cardiac remodeling by promoting differentiation of fibroblasts to myofibroblasts following myocardial infarction. During the past year, we showed that forced expression of MRTF-A in dermal fibroblasts stimulates contraction of a collagen matrix, whereas contractility of MRTF-A null fibroblasts is impaired under basal conditions and in response to TGF- β 1 stimulation. We also identified an isoxazole ring-containing small molecule, previously shown to induce smooth muscle α -actin gene expression in cardiac progenitor cells, as an agonist of myofibroblast differentiation. Isoxazole stimulates myofibroblast differentiation via induction of MRTF-A-dependent gene expression. The MRTF-SRF signaling axis is activated in response to skin injury, and treatment of dermal wounds with isoxazole accelerates wound closure and suppresses the inflammatory response. These results reveal an important role for MRTF-SRF signaling in dermal myofibroblast differentiation and wound healing and suggest that targeting MRTFs pharmacologically may prove useful in treating diseases associated with inappropriate myofibroblast activity.

Myocardial infarction (MI) leads to cardiomyocyte death, which triggers an immune response that clears debris and restores tissue integrity. In the adult heart, the immune system facilitates scar formation, which repairs the damaged myocardium but compromises cardiac function. In neonatal mice, the heart can regenerate fully without scarring following MI; however, this regenerative capacity is lost by P7. The signals that govern neonatal heart regeneration are unknown. By comparing the immune response to MI in mice at P1 and P14, we identified differences in the magnitude and kinetics of monocyte and macrophage responses to injury. Using a cell-depletion model, we determined that heart regeneration and neoangiogenesis following MI depends on neonatal macrophages. Neonates depleted of macrophages were unable to regenerate myocardia and formed fibrotic scars, resulting in reduced cardiac function and angiogenesis. Immunophenotyping and gene expression profiling of cardiac macrophages from regenerating and nonregenerating hearts indicated that regenerative macrophages have a unique polarization phenotype and secrete numerous soluble factors that may facilitate the formation of new myocardium. Our findings suggest that macrophages provide necessary signals to drive angiogenesis and regeneration of the neonatal mouse heart. Modulating inflammation may provide a key therapeutic strategy to support heart regeneration.

Obesity develops in response to an imbalance of energy homeostasis and whole body metabolism. Muscle plays a central role in the control of energy homeostasis through consumption of energy and signaling to adipose tissue. We reported previously that MED13, a subunit of the Mediator complex, acts in the heart to control obesity in mice. To further explore the generality and mechanistic basis of this observation, we investigated the potential influence of MED13 expression in heart and muscle on the susceptibility of *Drosophila* to obesity. We showed that heart/muscle-specific knockdown of MED13 or MED12, another Mediator subunit, and increases susceptibility to obesity in adult flies. To identify possible muscle-secreted obesity regulators, we performed

an RNAi-based genetic screen of 150 genes that encode secreted proteins and found that Wingless inhibition also caused obesity. Consistent with these findings, muscle-specific inhibition of Armadillo, the downstream transcriptional effector of the Wingless pathway, also evoked an obese phenotype in flies. Epistasis experiments further demonstrated that Wingless functions downstream of MED13 within a muscle regulatory pathway. Together, these findings reveal an inter-tissue signaling system in which Wingless acts as an effector of MED13 in heart and muscle and suggest that Wingless-mediated crosstalk between striated muscle and adipose tissue controls obesity in *Drosophila*. This signaling system appears to represent an ancestral mechanism for the control of systemic energy homeostasis.

B. MONTGOMERY PETTITT, CHAIR H-0037, The University of Texas Medical Branch at Galveston.

Solubility is a benchmark thermodynamic solution property for any solution, and we were able to make the first quantitative theoretical estimate of a peptide. The solubility limit of Gly₅ was calculated and compared with experimental values. We find the interactions driving peptide associations, which are the same as a liquid-liquid phase separation, are not predominantly hydrogen bonding. Instead, non-hydrogen bonding interactions between partially charged atoms on the peptide backbone allow the formation of carbonyl dipole-dipole and charge layering correlations that mechanistically stabilize the formation of large, stable peptide clusters. The hydration thermodynamics of an amino acid relative to the reference glycine or the hydration thermodynamics of a small-molecule analog of the side chain is often used to model the contribution to protein stability and solution thermodynamics. We also considered the reasons for successes and limitations of this approach by calculating and comparing the conditional excess free energy, enthalpy, and entropy of hydration of the isoleucine side chain in zwitterionic isoleucine, in extended penta-peptides, and in helical deca-peptides. Butane in gauche conformation served as a small-molecule analog for the isoleucine side chain. We found aspects of hydration thermodynamics are sequence context-sensitive. The context-sensitivity of hydrophobic and hydrophilic hydration and the addition of background contributions with energetics attributed to the side chain limit the ability of a single scaling factor, such as the fractional solvent exposure of the group in the protein, to map the component energetic contributions of the model compound data to their value in the protein.

LASZLO PROKAI, CHAIR BK-0031, University of North Texas Health Science Center.

In the grant year of 2013/2014, I published a fully developed procedure to explore the nitroproteome as part of Research Objective A. In particular, I described the chemistry applied to chemoprecipitation of nitropeptides, and developed specific guidelines for follow-up mass spectrometric analyses and bioinformatics focusing on nitroprotein identification and quantification. In addition, I have started new activities directed to analyses of reactive aldehyde species derived from oxidative stress-associated lipid peroxidation through isotope-coded derivatization. Specifically, our publication has been the first to characterize systematically the chromatographic isotope effect due to deuterium *versus* heavy-isotope substitution. Using proteomics, I have also initiated a project aimed at understanding the global role of specific lipids (phosphatidylglycerols) in cyanobacteria as a model organism. As part of my Research Objective B, I have gained supporting evidence through immunohistochemistry aided by the use of estrogen receptor-specific inhibitors that the para-quinol of estradiol is a brain-selective bioprecursor prodrug of the hormone. In pursuit of Research Objective C, I successfully employed the inhibition of tyrosine hydroxylase, an enzyme catalyzing the first and rate-limiting step in catecholamine biosynthesis, to induce experimental parkinsonism in an invertebrate (planarian) model, which could lead to further, neurochemistry-driven research on the dopaminergic control of movement and facilitate phenotypic drug discovery.

PETER J. ROSSKY, CHAIR F-0019, The University of Texas at Austin.

Fundamental research on the impact of an aqueous environment on biomolecular structure, on electronic states of complex molecular systems, and on nuclear quantum dynamics in condensed phase systems has been carried out. In the biophysical area, a long-term interest in hydration of biopolymer systems has continued. It has been demonstrated that an atomic-resolution scale for amino acid hydrophobicity resolves long-standing inconsistencies in understanding protein hydration using such scales and provides a dramatic improvement in the value of visualization of hydrophobicity from experimental structural results. In the area of electronic states, in collaboration with experimentalists, molecular modeling has explained the observed role of side chains on electronic states in an important class of semiconducting conjugated polymers. Again collaborating with experimentalists, a quantum nuclear dynamics algorithm has been implemented for analysis of observed dynamic structure factors in low temperature liquid hydrogen. The results show that theory can be used to reduce uncertainties in the measurements and hence enhance their value. Finally, in a series of papers, the equilibrium quantum structural and dynamic properties of water, primarily in low temperature clusters, has been examined. Of most interest, it has been demonstrated that there should be an easily measurable temperature dependent partitioning of H vs. D in cold clusters, which should allow IR spectral access to cluster temperature estimates. All of these projects are continuing.

JAMES C. SACCHETTINI, CHAIR A-0015, Texas A&M University.

Significant advancements have been achieved in the past year. Our interdisciplinary lab is continuing to increase its capabilities and efforts in drug discovery. We are focusing on several new targets and potential leads against *Mycobacterium tuberculosis*, cancer and other drug resistant pathogens. Most notably, we have expanded our structure-based drug discovery platform with special emphasis on two exciting projects for *M. tuberculosis* drug targets AccD6 and Pks13.

Our studies indicate that Acyl CoA carboxylase enzyme for *M. tuberculosis* are very important for cell envelope and lipid biosynthesis. Indeed disruption of this pathway leads to rapid cell death. We have determined the crystal structure of *Mtb* acyl-CoA carboxylase carboxyltransferase (AccD6) in

complex with several herbicide-based inhibitors, such as haloxyfop and quizalofop. We have used these structures to synthesize hundreds of analogs, many with very potent whole cell activity. Like the herbicides, our active compounds have low toxicity and outstanding PK. These are being readied for mouse efficacy studies.

Pks13 is a large multi-modular type I polyketide synthase (1733 aa) that is involved in mycolic acid biosynthesis, a known essential pathway in *M. tuberculosis*. We have identified a compound that selects for resistance mutations in the C-terminal thioesterase domain of Pks13. Through whole-genome sequencing, we were successful in making soluble enzyme and solving the crystal structure with the whole cell active HTS hit. Over 100 analogs have been synthesized and tested enzyme and *Mtb* growth activity and the crystal structure of complexes have been solved with the most critical inhibitors. Compound design was facilitated using the three-dimensional structures. Our best inhibitors to date have low nanomolar whole cell potency, good PK properties, no overall toxicity and are being prepared for efficacy testing in an animal model of *M. tuberculosis* infection.

Both of the aforementioned projects have been adopted as lead optimization projects, by the Bill and Melinda Gates Foundation's TB accelerator program.

GUSTAVO E. SCUSERIA, CHAIR C-0036, Rice University.

During the past year, we have continued to develop 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 wavefunction methods. The improvement of existing exchange-correlation functionals for density functional theory has remained an area of research in our group but was no longer central as in previous years. Our main efforts have focused on developing a very promising new wave function theory, Projected Quasiparticle Theory, for describing strong correlations. This novel method is applicable both to ground and excited states and the results continue to be very encouraging.

ERIC E. SIMANEK, CHAIR P-0008, Texas Christian University.

This report covers the fourth year of activities at Texas Christian University. Research highlights over the last period include:

1. Large dendrimers. Efforts to understand the factors that control solubility, limit size and retard reactivity were pursued and a description of these efforts is forthcoming. In short, microwave assisted reactions make the production of protein-sized molecules straightforward. Strategies to create virus-sized particles using organic and inorganic cores are ongoing. In collaboration with a Finnish group, the use of these dendrimers for patterning materials was pursued during this period.

2. Therapy. Anticancer efforts are now being supported by other funding agencies. The use of these materials as antimicrobials has commenced during this period.

Education efforts with the Pangea Mat & Cutter, a tool for teaching plate tectonics in middle school, are estimated to reach 100,000 students each year. These tools have been adopted broadly across the country. Carolina Scientific is a distributor. The Dance of the Continents has reached new scale with more than 750 actors participating in a single, four-school performance.

DENNIS W. SMITH, JR., CHAIR AT-0041, The University of Texas at Dallas.

This annual report was prepared by Bruce M. Novak, Dean, School of Natural Sciences and Mathematics, for Dennis W. Smith in *absentia*.

The funds from the Welch Foundation Chair 2 supported the research of Dr. Dennis Smith's group comprised of six PhD students, three undergraduates, one postdoc and two high school summer interns. Two of the graduate students, Babloo Sharma and Rajneesh Verma, completed and successfully defended their PhD dissertations in July 2013.

Dr. Smith has been on a leave-of-absence from the University for the 2013-14 academic year - the bulk of the period covered by this report. The Welch Chair two was vacated on January 1, 2014. It is my understanding the Robert A. Welch Foundation was kept informed throughout this transition. To maintain continuity, the funding for Dr. Smith PhD some of students continued through Spring 2014. The School of Natural Sciences and Mathematics in conjunction with the Department of Chemistry are formulating a search plan to fill this Welch Chair.

The Group's research interests and activities during this funding period included the synthesis, mechanism, structure/property relationships, and applications of polymeric materials and composites including: (1) fluoropolymers from aromatic trifluorovinyl ethers and other fluoroolefins for optical, energy conversion, and tailored surface applications, (2) polyarylene networks and carbon structures from micro and nano processable intermediates via bis-ortho-diyne arene (BODA) monomers, (3) renewable polymers based on aliphatic polyesters (e.g., PLA, PHA, and derivatives) and their applications in biomedical devices, (4) reground car tire rubber recycling via functionalization and composite formulation and carbonization, (5) novel carbon fiber precursor polymers based on copolymers with acrylonitrile, (6) thermally reversible crosslinkable resins for smart coatings, and (7) direct fluorination of materials for enhanced surface properties. In carrying out this work, collaborations with several UT Dallas faculties were developed and include D.J. Yang (UTD, Chemistry), Duncan MacFarlane (UTD, EE), Walter Voit (UTD, MSE), Ray Baughman (UTD, Chemistry), John Ferraris (UTD, Chemistry) and Yves Chabal (UTD, MSE). Seven publications have been included in this report that covers four of these seven focus areas:

(1) **Fluoropolymers:** The fluoropolymer work is a continuation of a long-standing focus of the Smith Group. Publications in this area include two articles (optoelectronic applications) one article (new polymer compositions), and one article (modification of surface properties using FOSS with fluorinated side chains).

(4) **Ground Tire Composites:** An article discusses the use of functionalized GIRT in epoxy matrices.

(5) **Carbon Precursor Polymers:** Progress in the area of carbon fiber precursor materials include one publication, wherein these acrylonitrile precursors are modified for smart NO release from sutures.

(7) **Direct Fluorination:** Progress in the direct fluorination of graphene oxide (GO) is reported in one publication.

JOHN L. SPUDICH, CHAIR AU-0009, The University of Texas Health Science Center at Houston.

We continued to make major progress on the chemistry of rhodopsin light-gated channels (channelrhodopsins (ChRs)) used in the new biotechnology of optogenetics, the control of cellular (typically neuronal) membrane potential with light. We identified a new channelrhodopsin, PsChR, a phototaxis receptor in the alga *Platymonas subcordiformis* that exhibit ~3-fold higher unitary conductance and greater relative permeability for Na⁺ ions, compared to the most frequently used channelrhodopsin-2 from *Chlamydomonas reinhardtii* (CrChR2). Photocurrents generated by PsChR in HEK293 cells showed lesser inactivation and faster peak recovery than those by CrChR2. Their maximal spectral sensitivity is at 440 nm, making PsChR the most blue-shifted channelrhodopsin so far identified. PsChR mediated sufficient light-induced membrane depolarization in cultured hippocampal neurons to trigger reliable repetitive spiking at the neurons' upper threshold frequency. At extended times spiking probability decreases less with PsChR than with CrChR2 because of the former's faster recovery. The greater activity of PsChR facilitates the study of structure/function relationships in ChRs. In particular we made progress on the nature of spectral tuning of these molecules. A key factor known from earlier work is that the effective charge of two conserved carboxylic acid residues in the retinylidene photoactive site of rhodopsins largely determines their color (i.e. their absorption spectrum). We found that highly effective ChRs, including PsChR and CrChR2, contain a lysyl residue in transmembrane helix B that modulates the pKa values of the two active site carboxylic acid residues. An Arg residue in helix C plays this role in other classes of microbial rhodopsin, revealing a different organization of the photoactive site electrostatic interactions in ChRs.

DOUGLAS M. STOCCO, CHAIR BI-0028, Texas Tech University Health Sciences Center.

In 2013, our laboratory engaged in several lines of investigation. We have described the role of members of the retinoid family in the acute regulation of StAR expression and steroid hormone biosynthesis. We demonstrated that all-trans retinoic acid (atRA) was capable of enhancing StAR expression, but not its phosphorylation (P-StAR), and progesterone production in Leydig cells. Activation of the protein kinase A (PKA) cascade, by (Bu)₂cAMP or type I/II PKA analogs, synergistically enhanced retinoid- responsive StAR, P-StAR, and steroid levels. Targeted silencing of endogenous RAR α and RXR α , with siRNAs, resulted in decreases in 9-cis RA-stimulated StAR and progesterone levels. Deletion and mutational analyses in the 5'-flanking region of the StAR gene demonstrated the relevance of the -254/-1 bp region in retinoid responsiveness. An oligonucleotide probe encompassing an RXR/liver X receptor recognition motif, located within the -254/-1 bp region, was found to specifically bind MA-10 nuclear proteins in EMSAs. Transcription of the StAR gene by atRA and (Bu)₂cAMP was influenced by phosphorylation of the cAMP response-element binding protein (P-CREB). These findings provided novel insight into the regulation of retinoid-mediated StAR expression and steroid biosynthesis. We were also engaged in collaborative studies that definitively demonstrated that the translocator protein (TSPO), a protein long purported to be indispensable in steroid biosynthesis is not involved in steroidogenesis neither in cell culture model systems nor in the whole animal, findings that have refuted 25 years of dogma concerning this protein.

CHERYL LYN WALKER, CHAIR BE-0023, Texas A&M University System Health Science Center.

1) Peroxisomes are highly metabolic, autonomously replicating organelles that generate ROS as a by-product of fatty acid β -oxidation. Consequently, cells must maintain peroxisome homeostasis, or risk pathologies associated with too few peroxisomes, such as peroxisome biogenesis disorders, or too many peroxisomes, inducing oxidative damage and promoting diseases such as cancer. We report that the PEX5 peroxisome import receptor binds ATM and localizes this kinase to the peroxisome. In response to ROS, ATM signaling activates ULK1 and inhibits mTORC1 to induce autophagy. Specificity for autophagy of peroxisomes (pexophagy) is provided by ATM phosphorylation of PEX5 at Ser141, which promotes PEX5 mono-ubiquitination at K209 by the peroxisome E3 ligase PEX2/10/12. Ubiquitinated-PEX5 is recognized by the autophagy adapter protein p62, directing the autophagosome to peroxisomes to induce pexophagy. These data reveal an important new role for ATM signaling at the peroxisome as a sensor of ROS that maintains peroxisome homeostasis.

2) SEND, a historic methyltransferase is altered in kidney (and other) cancers. Our work on SEND has taken an exciting new direction with our recent discovery that SEND has a novel function as a microtubule methyltransferase required for genomic stability. We found that in addition to "writing" the epigenetic histone H3 lysine 36 trimethyl (H3K36me3) marks, SEND methylates microtubules during mitosis. SEND microtubule methylation is required for spindle function, proper chromosome segregation, and abscission during cytokinesis. Based on these and other data, we propose that SEND loss contributes to the cancer phenotype by increasing genomic stability.

STEVEN WEINBERG, CHAIR F-0014, The University of Texas at Austin.

The scientific work of Steven Weinberg during 2013-2014 has centered on a new approach to quantum mechanics, in which the description of physical states is based on the density matrix rather than the state vector. This has the advantage of avoiding the "action at a distance" problems that worried Einstein, and it opens up new ways that physical systems may respond to symmetry transformations. Talks on this work have been given at the University of Texas, and the Kavli Institute for Theoretical Physics in Santa Barbara; a paper has been posted to the quant-ph archive (1405.3483) and submitted to the *Physical Review A*; and another paper is in preparation.

THEODORE G. WENSEL, CHAIR Q-0035, Baylor College of Medicine.

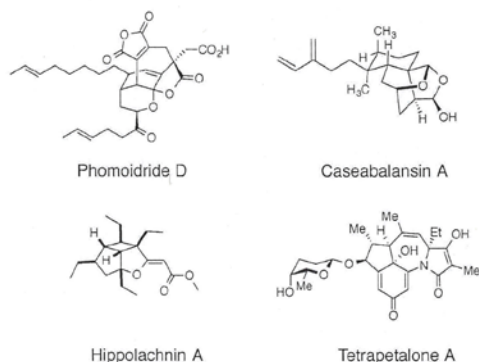
We have continued our work on structure and function of G-protein coupled receptors by engineering and testing many double mutants of the D2 dopamine receptor using residues of evolutionary importance identified by the Evolutionary Trace algorithm to be functionally coupled in evolution. We have identified double mutants, whose quantitative properties (ligand affinity, ligand potency, ligand efficacy) combine in a non-linear way on a free energy scale, confirming functional coupling. We have also thoroughly characterized the specificity of all three groups of metabotropic glutamate receptors, and discovered surprising new properties: 1) Group I receptors are weakly inhibited by endogenous neurotransmitter L-serine-O-phosphate, and Group II receptors are strongly inhibited by it. 2) Group I receptors can activate Gi-class G proteins as well as Gq-class G proteins. 3) Mutating a single amino acid residue, identified by computational docking from glutamine to lysine greatly enhances the affinity of mGluR7 for L-serine-O-phosphate. We have purified recombinant TRPM1, an ion channel essential for night vision, and determined its structure by cross-linking, native electrophoresis, and cryo-electron microscopy to be a homodimer. We have developed methods for purifying large quantities of the ion channel TRPV2 in detergent, and stabilizing it with amphipoles, incorporating it into lipid vesicles, where we have proven it to be functional, or setting up crystallization trials. We have also begun collection images of purified TRPV2 in amphipole by cryo-electron microscopy using a direct electron detection camera in order to determine its structure at high resolution.

PETER G. WOLYNES, CHAIR C-0016, Rice University.

The Bullard-Welch Chair supports trips of group members working on Welch funded projects as well as participation in several meetings by Peter Wolynes. Graduate student A. Wisitorsak was supported by the Chair until his his graduation in May 2014. He will join the physics faculty of Mahidol University in Thailand.

JOHN L. WOOD, CHAIR AA-0006, Baylor University.

The Wood group is currently comprised of four graduate students and three postdoctoral fellows. Efforts in the during the current funding period have been directed toward the synthesis of four natural product, including: A) Phomoidride D, a naturally occurring inhibitor of RAS farnesyl transferase and squalene synthase; B) Caseabalansin A, a natural product with activity against PC3 tumor cells; C) Hippolachnin A, a natural product with activity against fungal meningitis, and; D) Tetrapetalone A, a naturally occurring lipoxygenase inhibitor. The structures of these compounds are illustrated below.



KAREN L. WOOLEY, CHAIR A-0001, Texas A&M University.

A productive research, education and training program involving the design, preparation and study of unique polymer materials is supported by the Welch Foundation grant. The W. T. Doherty-Welch Chair in Chemistry at Texas A&M University supports significant portions of the infrastructure that is directed toward an innovative mission to educate and train a diverse community of scholars (four undergraduate students, 23 Ph.D. students, six postdoctoral associates, and four senior scientists), each conducting research to advance the fundamental knowledge and societal application of functional polymer materials. Supplemental support comes from grants from the National Institutes of Health! the National Science Foundation, the Office of Naval Research and Dow Corporation. Importantly, the entire research program involves a motivation to extend the synthetic control of organic chemistry toward increasingly complex and functional materials over many dimensions, often by employing hierarchical approaches, and it relies on combinations of organic chemistry, physical chemistry, biology and engineering. Research advances have included advances with well-defined molecular brush block copolymers having intricate compositions and structures toward ultra-high resolution photoresists for microelectronics patterning, hybrid organic polymer-inorganic magnetic nanoparticle assemblies designed for environmental clean-up that are capable of capturing 10× their mass in crude oil with magnetic recovery, extension of shell crosslinked knedel-like nanoparticles as dual imaging and therapeutic delivery vessels for treatment of cancer, acute lung injury and lung infectious diseases, anti-biofouling coatings that present surface complexities and exhibit modes of passive and active foulant deterrents for employment in the marine environment, and degradable polymers derived from renewable resources and that undergo breakdown to release biologically-beneficial and environmentally-

resorbable natural product small molecules. Research efforts have led to 26 peer-reviewed published articles, two articles in press, and six manuscripts submitted for publication, currently undergoing peer review. The Welch Foundation chair is gratefully acknowledged for its contribution to each of these advances, by serving as seed funds, and supporting tuition expenses, instrumentation access fees, and materials and supplies costs.

CHAIR AQ-0039, The University of Texas Health Science Center at San Antonio.

Due to budgetary limitations within the Department, we had not launched a search last year to fill this chair. These resolved themselves over the last year with several retirements and the addition of new grants within the department. Hence, we have constituted a search committee and obtained approval from the School of Medicine to move ahead with an international search this year.

The committee is chaired by Dr. Bruce Nicholson, and has membership from Biochemistry (Welch Chair - Bettie Sue Masters; Welch supported investigators - Paul Fitzpatrick, John Hart, Andy Hinck; plus Phil LoVerde), other departments (LuZhe Sun - CTRC and Cell and Structural Biology), schools (Ken Hargreaves - CTSA and Dental School), and campuses (Doug Frantz - Chemistry at UTSA).

We opened the search in January, and have received 24 applications. We have also reached out to individuals and added three to four additional applicants to the pool. After rigorous review, we have invited three applicants in for interviews to this point (one subsequently withdrew prior to the interview for personal reasons). We propose to move forward with this process and have a final candidate recruited during the Fall.

We have utilized some Welch resources for the recruiting efforts (\$5,476), and some more will be expended, but the vast majority of the significantly accrued interest account (\$644K) will be used to contribute to the start-up costs for the incoming recruit. These amounts will be leveraged maximally with additional resources from UT STARS and CPRIT funds in order to recruit the best candidate.

PUBLICATIONS BY PRINCIPAL INVESTIGATORS REPORTED DURING 2013 – 2014

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