



**September 9, 2013  
Indianapolis, Indiana  
246th ACS National Meeting**

# AEI Poster Session Grid 2013

*Poster #	Name	AGFD	ANYL	BIOL	BIOT	CARB	CATL	CELL	CHAL	CHED	COLL	COMP	ENFL	ENVR	FUEL	GEOC	INOR	MEDI	NUCL	ORGN	PHYS	PMSE	POLY	SCHB	TOXI	
1	<a href="#">S. Martínez-Monteaqudo</a>	•																								
2	<a href="#">B. Bogusz</a>	•	•																							
3	<a href="#">K. Bantz</a>		•	•																						
4	<a href="#">F. Camacho-Alanis</a>	•		•					•	•																
5	<a href="#">C. Daniels</a>	•																			•					
6	<a href="#">F. Deiss</a>	•	•																							
7	<a href="#">L. Demoranville</a>	•																		•						
8	<a href="#">M.S. Devadas</a>	•												•			•						•			
9	<a href="#">J. Jenkins</a>	•											•													
10	<a href="#">C. Rainey</a>	•																								•
11	<a href="#">G. Stokes</a>	•																					•			
12	<a href="#">H. Tavassol</a>	•									•	•											•			
13	<a href="#">S. Hattan</a>	•																								
14	<a href="#">E. Walker</a>	•																								
15	<a href="#">G. Liu</a>		•																							
16	<a href="#">A. Garg</a>		•																			•				
17	<a href="#">J. Gavenonis</a>		•															•								
18	<a href="#">T. Neumann</a>		•											•												
19	<a href="#">J. Pollock</a>		•																				•			
20	<a href="#">Y. Tal-Gan</a>		•																•	•						
21	<a href="#">A. Weerasinghe</a>		•																							
22	<a href="#">J. Wu</a>	•	•																							
23	<a href="#">M. Anzovino</a>										•															
24	<a href="#">Withdrawn</a>																									
25	<a href="#">S. Dolai</a>		•									•									•					•
26	<a href="#">J. Jankolovits</a>										•			•							•				•	
27	<a href="#">S. Perry</a>			•									•													
28	<a href="#">A. Akimov</a>													•				•								•
29	<a href="#">J. Baker</a>																	•								
30	<a href="#">R. Coleman</a>			•														•								
31	<a href="#">H. Liu</a>																	•								•
32	<a href="#">P. Kekenes-Huskey</a>																									•
33	<a href="#">S. Kim</a>			•														•				•			•	
34	<a href="#">A. Kutana</a>																	•								•
35	<a href="#">S. Nichols</a>				•													•				•				
36	<a href="#">P. Schyman</a>																	•								•
37	<a href="#">D. Sindhikara</a>					•												•				•			•	
38	<a href="#">E. Sproviero</a>								•									•	•							•
39	<a href="#">R. Swift</a>						•																			•

\*Poster numbers may change due to late withdrawals

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40	<a href="#">S. Fegade</a>											•		•													
41	<a href="#">G. LeBlanc</a>	•										•	•	•													
42	<a href="#">K. Mudiyanselage</a>									•		•												•			
43	<a href="#">C. Patridge</a>										•													•			
44	<a href="#">C. Adams</a>												•														
45	<a href="#">R. Hansen</a>	•											•														
46	<a href="#">D. Stewart</a>	•							•				•														
47	<a href="#">J. Atchison</a>													•											•		
48	<a href="#">L. Zhang</a>											•	•		•	•											
49	<a href="#">T. Liu</a>																										
50	<a href="#">P. Adelani</a>											•	•				•										
51	<a href="#">L.A. Ariyadasa</a>															•							•				
52	<a href="#">A. Basner</a>																•					•			•		
53	<a href="#">J. Brdoch</a>																	•									
54	<a href="#">T. Gardner</a>																	•									
55	<a href="#">S. Dorazio</a>																	•									
56	<a href="#">J. Scepaniak</a>																	•									
57	<a href="#">J. Hahn</a>	•																•					•				
58	<a href="#">K. Higgins</a>	•																•									
59	<a href="#">S. Kilyanek</a>							•										•									
60	<a href="#">S. Lohse</a>	•								•								•									
61	<a href="#">A. Mukherjee</a>	•																•						•			
62	<a href="#">V. Neti</a>																	•									
63	<a href="#">S. Vaddypally</a>																	•						•			
64	<a href="#">U. Williams</a>																	•									
65	<a href="#">A. Chatterjee</a>										•							•	•								
66	<a href="#">O. Cojocaru</a>												•					•	•								
67	<a href="#">J. Zhou</a>	•																•									
68	<a href="#">S. Chamberland</a>																	•	•								
69	<a href="#">S. Dawn</a>			•															•								
70	<a href="#">T. Fisher</a>																			•							
71	<a href="#">N. Hussain</a>																			•							
72	<a href="#">L. Miller</a>		•																•	•							
73	<a href="#">M. Ratnikov</a>																			•							
74	<a href="#">K. Roy</a>		•																	•					•	•	
75	<a href="#">B. Saha</a>														•			•	•	•							
76	<a href="#">A. Schafer</a>																			•							
77	<a href="#">B. Taylor</a>													•					•		•						
78	<a href="#">K. Waynant</a>																					•	•	•			

\*Poster numbers may change due to late withdrawals

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79	<a href="#"><u>J. Yi</u></a>						•						•				•									
80	<a href="#"><u>M. Chen</u></a>		•										•								•					
81	<a href="#"><u>B. Ivanov</u></a>									•							•				•	•				
82	<a href="#"><u>Y. Li</u></a>		•																	•	•					
83	<a href="#"><u>G. Lindberg</u></a>											•			•							•				
84	<a href="#"><u>J. Newby</u></a>		•																			•				
85	<a href="#"><u>C. Ragain</u></a>			•						•												•				
86	<a href="#"><u>A. Raiqoza</u></a>											•										•				
87	<a href="#"><u>D. Swenson</u></a>											•										•				
88	<a href="#"><u>B. Wong</u></a>											•										•				
89	<a href="#"><u>L. Xu</u></a>											•								•	•	•				
90	<a href="#"><u>M. Kiechel</u></a>						•	•													•	•				
91	<a href="#"><u>D. Priftis</u></a>																				•	•				
92	<a href="#"><u>F. Ren</u></a>													•								•				
93	<a href="#"><u>B. Ulery</u></a>					•																•	•			
94	<a href="#"><u>J. Lott</u></a>																					•	•			
95	<a href="#"><u>B. Fors</u></a>																			•		•	•			
96	<a href="#"><u>A. Abbaspourrad</u></a>						•					•								•			•			
97	<a href="#"><u>L. Xu</u></a>						•	•											•						•	

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## AEI 2013

### Biographical Sketches

**1. Sergio I. Martinez-Monteagudo;** Department of Agricultural, Food and Nutritional Science, University of Alberta, 410 Agriculture/Forestry Centre, T6G 2P5, Edmonton, AB, Canada; 780-761-5193; [simartin@ualberta.ca](mailto:simartin@ualberta.ca); Autonomous University of Chihuahua (B.Sc., 2003; M.Sc., 2005); University of Alberta (Ph.D., anticipated Sep 2013), Dr. Marleny Saldana, Kinetics studies of chemical reactions in high-pressure sterilized milk.

My primary goal is to become an academic at a research-oriented university. My interest is the application of emerging technologies, such as high-pressure sterilization, to develop functional foods enriched with bioactive compounds (conjugated linoleic acid and antioxidants). Additionally, the way in which chemical reactions and quality parameters in foods are affected by high-pressure sterilization is another of my research interests. I believe that finding alternatives for obtaining healthier foods is one way to open new markets. Over three years, I have served as a teaching assistant for the course unit operations for food preservation, plus a forth-year undergraduate course.

Abstract Title: *High pressure sterilization of milk rich in conjugated linoleic acid*

AGFD Division

**2. Brandon Bogusz;** Department of Food Science, Rutgers University, 65 Dudley Road, New Brunswick, NJ 08901; [bogusba05@juniata.edu](mailto:bogusba05@juniata.edu); Juniata College (B.S, 2008); Rutgers University (Ph.D., anticipated, 2014), Dr. Karen Schaich, Monitoring volatile products of alternate lipid oxidation pathways.

I am seeking a faculty position at a primarily undergraduate institution that emphasizes excellence in undergraduate education and also values undergraduate research. I have taught undergraduate lab sections in analytical chemistry and Principles of Food Science while also mentoring one undergraduate student. I have also developed and taught a 1.5 credit course, titled “Introduction to Scientific Research,” so that first-year students can learn about how research is conducted. My research will focus on using chromatography to learn more about the kinetics, mechanisms, and oxidative stability of foods.

Abstract Title: *How do lipids oxidize in foods?*

AGFD, ANYL Divisions

**3. Kyle Christine Bantz;** Biomedical Engineering Department, Northwestern University, 2145 Sheridan Rd., Tech E310, Evanston, IL 60208; 847-467-2957, [kyle.bantz@northwestern.edu](mailto:kyle.bantz@northwestern.edu); Cornell College (B.A., 2006); University of Minnesota (Ph.D., 2011), Prof. Christy L. Haynes, Development and application of partition layer-modified surface-enhanced Raman scattering (SERS) sensors for complex mixture analysis; Postdoctoral Fellow at Biomedical Engineering Department, Northwestern University, (2012–present), Prof. Milan Mrksich, Understanding phosphatase evolution and influence in cellular states.

I am seeking a faculty position at a primarily undergraduate four-year college or university with a strong emphasis on undergraduate education and research. I have two years of experience leading nonmajor general chemistry undergraduate and analytical laboratories. Additionally, I assisted in teaching an undergraduate analytical course and a course on current topics in biosensors, both of which included preparing lectures, writing homework, and exams. I have also mentored six undergraduate students, two of whom received publications from their research. My research interests are interdisciplinary and focus on applying traditional analytical and bioanalytical tools to develop novel biosensors.

Abstract Title: *Understanding the evolutionary relationship of protein tyrosine...*

ANYL, BIOL Divisions

**4. Fernanda Camacho Alanis;** Tempe, Arizona 85281; 434-465-8440, [facamach@asu.edu](mailto:facamach@asu.edu); National Autonomous University of Mexico (B.S., 2001; M.S., 2006); University of Virginia (Ph.D., 2010), won two research awards [Adviser and research topic not provided]; Postdoctoral Research Associate at Arizona State University (2010–present), part of the committee for two Honors theses, Prof. Alexandra Ros, Nanostructured microfluidic devices for biomolecular applications.

I seek a tenure-track faculty position in materials science, chemical engineering, or chemistry to establish a funded research program and mentor students. Accomplishments include 14 publications and 17 presentations at national and international conferences. My research interests are synthesis, fabrication, and characterization of nanomaterials applied to biotechnology, energy, and microelectronics. My teaching interests include nanomaterials, electrochemistry, separation processes, and solid-state chemistry. I have mentored graduate and undergraduate students and was a TA for undergraduate and graduate classes in general chemistry, IC fabrication, and analytical chemistry. Finally, I would also consider tenure-track faculty positions at teaching universities or colleges.

Abstract Title: *Protein dielectrophoresis probed with insulator based devices...*

ANYL, BIOT, CHED, CHAL Divisions

**5. Charlisa R. Daniels;** Department of Chemistry, Trinity University, 1 Trinity Place, San Antonio, TX 78212; 210-999-7842, [cdaniels@trinity.edu](mailto:cdaniels@trinity.edu); Agnes Scott College (B.A., 2005); Rice University (Ph.D., 2012), Dr. Christy F. Landes, Monitoring transport at interfaces of tunable soft surfaces; Postdoctoral Associate at Trinity University (2012–present), Dr. Michelle Bushey, Characterizing lauryl acrylate porous polymer monoliths using HPLC and CEC.

I seek a faculty position at an undergraduate institution that values both teaching and research. My experience involving undergraduates includes lecturing general and analytical chemistry classes, teaching organic and analytical chemistry labs, and developing general and physical chemistry recitations. Furthermore, I aspire to develop courses that allow students to realize the intersection of chemistry and their extracurricular interests. Finally, I collaborate and publish with undergraduates. I plan to develop an interdisciplinary research program focusing on the synthesis, characterization, and utility of tunable polymers. I am excited to expand on my experience with undergraduates, providing a well-rounded and innovative chemistry education.

Abstract Title: *Characterizing Lauryl acrylate porous polymer monoliths using HPLC*

ANYL, PHYS Divisions

**6. Frédérique Deiss;** Department of Chemistry, University of Alberta, Edmonton, AB T6G 2G2, Canada; 617-459-5034 (U.S.) or 587-778-0270 (Canada), [deiss@ualberta.ca](mailto:deiss@ualberta.ca); Ecole Nationale Supérieure de Chimie et Physique de Bordeaux, France (Ingénieur/Master's degree, 2006); University of Bordeaux, group NanoAnalytical Systems (Ph.D., Chem–Physics, 2009), Prof. Neso Sojic, Multiplexed electrochemical biosensor arrays on optical fiber bundle; Postdoctoral Fellow at Harvard University (2009–2012), Prof. George M. Whitesides, Low-cost point-of-care diagnostic tools, paper-based glucometer test strip for multiple analytes detection, platform for drug testing on 3-D cell cultures in paper array; Postdoctoral Researcher at University of Alberta (2012–present), Dr. Ratmir Derda, Paper-based bioanalytical (microbiological) platforms.

In a Ph.D.-granting institution, I want to establish a strong research program to develop original bioanalytical and electrochemical platforms. One of my proposal ideas won the Canadian Innovation Challenge SENTINEL EXCELerator award (May 2013), confirming my ability to be creative, present my projects, and be aware of current health issues, which will help get external funding. One or more aspects of my future group will attract motivated students: (i) developing new bioanalytical systems for analyte detection and quantification; (ii) working at the interface of Chemistry–Physics–Biology; (iii) incorporating those systems into simple, point-of-care diagnostic devices that will improve global and public health.

Abstract Title: *Development of bioanalytical platforms using original substrates such...*

ANYL, BIOL Divisions

**7. Leonard Demoranville;** Chemistry Program, Centre College, 600 W. Walnut St., Danville, KY 40422; 859-238-6066, [leonard.demoranville@centre.edu](mailto:leonard.demoranville@centre.edu); Eastern Nazarene College (B.S., 2003); University of Maryland College Park (Ph.D., 2010), Alice Mignerey, Evaluation of mass filtered, time dilated, time-of-flight mass spectrometry; NSF Postdoctoral Fellow at National Institute of Standards and Technology, Greg Gillen, Development of test materials and protocols for trace drug detection using ion mobility spectrometry; [http://www.centre.edu/faculty\\_staff/demoranville\\_leonard.html](http://www.centre.edu/faculty_staff/demoranville_leonard.html).

As a visiting professor, I am refining how I create a classroom environment that facilitates learning. Using a wide variety of active learning techniques, from think-pair-share and clickers to group and POGIL style activities, I seek to guide students toward appropriate learning goals. While at Centre, two students in my laboratory are developing advanced protocols for using ion mobility spectrometers in contraband screening at border crossings and prisons and in clandestine lab remediation. I use undergraduate research to deepen students' understanding of chemistry by applying classroom knowledge while developing an understanding of research processes.

Abstract Title: *Nitrates in the environment: Using the analytical chemistry laboratory...*

ANYL, NUCL Divisions

**8. Mary Sajini Devadas;** Department of Chemistry and Biochemistry, University of Notre Dame, 251 Nieuwland Science Hall, Notre Dame, IN 46556; [mdevadas@nd.edu](mailto:mdevadas@nd.edu); Bharathiar University (B.S., 1997; M.S., 1999; M.Phil. 2001); Western Michigan University (Ph.D., Chem, 2012), Dr. Ekkehard Sinn, Optical and electrochemical properties of fluorophore-modified quantum-sized gold clusters; Postdoctoral Researcher at University of Notre Dame (April 2012–present), Dr. Gregory V. Hartland, Single nanomaterial dynamics and development of novel spectroscopic techniques, such as optical trapping and spatial modulation spectroscopy besides transient absorption using ultrafast lasers; synthesis of 1-D and 2-D nanomaterial.

I am interested in developing material for light harvesting devices and catalysis using noble metal composite material. Secondly, I am interested in designing multifunctional nanosized metal–organic hybrid materials for multimodal noninvasive molecular imaging and detection. The agents will target to biomarkers of certain diseases, particularly neurodegenerative diseases such as Alzheimer's. I am interested in teaching and directing research at a four-year college or regional comprehensive university.

Abstract Title: *Single nanomaterial dynamics and imaging of gold spheres and plates*

ANYL, PHYS, INOR, ENVR Divisions

**9. Judith L. Jenkins;** 1306 E. University Blvd., Dept. of Chemistry, Tucson, AZ 85721; 309-299-0308, [judyj@email.arizona.edu](mailto:judyj@email.arizona.edu); Knox College (B.A., Chem, 2002; B.A., Secondary Ed, 2002); University of Arizona (Ph.D., Chem, 2012), Dr. Neal R. Armstrong, Spectroscopic and spectroelectrochemical characterization of fundamental interfacial charge transfer processes relevant to efficient solar energy conversion; Postdoctoral Researcher at the University of Arizona (2012–present), Dr. S. Scott Saavedra, Transient absorbance spectroscopy of novel chromophores in solution and on transparent electrode surfaces.

I am seeking a faculty position at a primarily undergraduate institution or a teaching-track position at a Research I institution. As an analytical chemist, my research interests focus on materials related to energy conversion (solar electricity, solar fuels, and batteries), and I look forward to welcoming undergraduate students into spectroscopic and electrochemical research efforts. I will teach students (majors and nonmajors alike) how molecular-level chemistry is critically relevant in our day-to-day existence and in addressing our growing needs for sustainable energy conversion technologies.

Abstract Title: *Photochemistry of chromophore/transparent conductive oxide interfaces...*

ANYL, ENFL Divisions

**10. Christina Rainey;** Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis, 402 N. Blackford St. LD 326, Indianapolis, IN 46202; [clrainey@iupui.edu](mailto:clrainey@iupui.edu); Wright State University (B.S., Chem, 2009); Purdue University at Indianapolis (Ph.D., Analyt Chem, anticipated 2013), Dr. John V. Goodpaster, Analysis of tobacco and tobacco usage in human hair.

My academic objectives are to teach analytical and forensic chemistry at a four-year university. My research interests include developing methodology to evaluate samples of forensic relevance. I have been a teaching assistant for undergraduate chemistry labs such as general chemistry, analytical chemistry, and instrumental analysis. Additionally, I have mentored undergraduate and high school students assisting in my graduate research. My teaching and mentoring experiences have prepared me to teach at a university level. I am particularly interested in teaching forensic chemistry and developing new courses and labs that will excite students about analytical chemistry.

Abstract Title: *Optimization of nicotine analysis using solid phase microextraction*

ANYL, TOXI Divisions

**11. Grace Y. Stokes;** Department of Chemistry, University of Utah, 315 S. 1400 E. Rm. 2020, Salt Lake City, UT 84108; [gystokes@chem.utah.edu](mailto:gystokes@chem.utah.edu); Stanford University (B.S., 2002), Northwestern University (Ph.D., 2009), Prof. Franz M. Geiger, Heterogeneous ozone oxidation reactions of olefins on silica substrates monitored by SFG vibrational spectroscopy; Dreyfus Environmental Postdoctoral Fellow at Johns Hopkins University (2009–2011), Prof. Alan T. Stone (Envr Eng) and Prof. Justine P. Roth (Chem), Oxidation of lignin-like organics by dissolved manganese(III) complexes; Postdoctoral Researcher at University of Utah (2011–present), Prof. John C. Conboy, Drug-cell membrane interactions studied by nonlinear optical spectroscopies; [www.gystokes.com](http://www.gystokes.com).

I would like to direct undergraduate and master's degree level students in studying the kinetics, thermodynamics, and organic mechanisms that govern interactions between emerging organic pollutants (such as hormone-based pharmaceuticals and personal care products) and environmentally relevant oxide surfaces. Our work will provide a fundamental understanding of adsorption, transport, and heterogeneous reactivity relevant to biogeochemistry. My doctoral coursework and postdoctoral research experiences have prepared me to teach classes in bioanalytical, physical, and environmental chemistry.

Abstract Title: *Using nonlinear optical spectroscopies to elucidate surface adsorption...*

PHYS, ANYL Divisions

**12. Hadi Tavassol;** Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana IL, 61801; [tavasso2@illinois.edu](mailto:tavasso2@illinois.edu); Sharif University of Technology (B.S., 2006); Northern Illinois University (M.S., 2009); University of Illinois at Urbana-Champaign (Ph.D., 2014), Prof. Andrew Gewirth, Interfacial processes in Li-ion batteries.

My research will focus on the characterization and control of electrochemical processes in interfaces and molecular systems. These processes are responsible for the performance and properties of important reactions in energy storage and electrocatalysis. A combination of in situ and ex situ spectroscopy, spectrometry, and structure probing techniques will be used for such studies. My teaching experience includes instructing electrochemistry and analytical chemistry laboratory courses, as well as mentoring undergraduate and visiting students in research.

Abstract Title: *Interfacial processes in Li ion batteries*

ANYL, ENFL, PHYS, COLL Divisions

**13. Stephen J. Hattan;** Senior Scientist, Virgin Instruments Corp., Sudbury, MA 01776; 857-719-1912, shattan64@netzero.net; U.S. Army Academy of Health Sciences, Fort Sam Houston, TX (Radiographic Tech, 1985); Saint Anselm College, Manchester, NH (B.S., Chem, 1988); University of New Hampshire, Durham (Ph.D., Analyt Chem, 1996), Dr. N. Dennis Chasteen, Purification and characterization of an extrapallial fluid protein from the mollusk, *Mytilus edulis*; Research Associate at NY State Dept. of Health (1997), Dr. Robert Trimble, Carbohydrate characterization by NMR; Research Associate at Whitehead Institute, MIT (1999), Dr. Paul Matsudaira, Protein characterization/sequencing; Senior Scientist at Applied Biosystems/Celera Proteomic Research Center (2000–2005); Senior Scientist at Virgin Instruments Corporation, Sudbury, MA (2006–present), SBIR grant 1 R43 GM079833-01, “New Separations for MALDI-TOF Mass Spectrometry.”

Recent research has focused on innovative ways for integrating protein separations with MALDI mass spectrometry for proteomic analyses. Innovations include a 3-dimensional MALDI plate for LC-MALDI workflows, bi-functional membrane for SDS-PAGE/MALDI interface and immobilized enzyme substrates for paper and thin-layer chromatography/MALDI. I wish to continue research in this area with expansion into green or sustainability methodology and practice. I am keenly interested in teaching (chemistry, analytical chemistry, biochemistry, and special topics). I have a strong background in academic and industrial research. I have instructed courses in the military and received a teaching excellence award in graduate school.

Abstract Title: *Innovative strategies for coupling separations with MALDI mass...*

ANYL Division

**14. E. Kate Walker;** Austin College, Department of Chemistry and Biochemistry, 900 N. Grand Avenue, Suite 61652, Sherman, TX, 75090; [kawalker@austincollege.edu](mailto:kawalker@austincollege.edu); The University of Texas at Dallas (B.S., Biochem & Molecular Bio, 2007), Dr. Paul Pantano, Materials characterization to assess cytotoxicity of carbon nanotubes; The University of Texas at Austin (Ph.D., Chem, 2012), Dr. Keith J. Stevenson and Dr. David A. Vanden Bout, Transparent carbon electrodes for spectroelectrochemical studies; Visiting Assistant Professor of Analytical Chemistry at Texas Wesleyan University (2012–2013); Visiting Assistant Professor of Chemistry at Austin College (2013–2014).

I am interested in combined technique approaches to investigate materials at the nano and bulk levels, with research students gaining experience in materials science, nanotechnology, electrochemistry, and spectroscopy. As a professor at Texas Wesleyan and a teaching assistant at UT Austin, I managed and mentored students as they developed independent research projects on a variety of instruments. My teaching experience includes general chemistry, analytical chemistry, graduate surface science, and science for nonmajors courses. I am interested in a tenure-track position at an institution that values excellence in both teaching and research, with a preference for a primarily undergraduate institution.

Abstract Title: *Spectroelectrochemical studies utilizing carbon optically...*

ANYL Division

**15. Gang Liu;** Laboratory of Biometrology and Bioanalysis, Department of Chemistry and Ionizing Radiation, Shanghai Institute of Measurement and Testing Technology (SIMT), 1500 Zhangheng Road, Shanghai (201203); [liug@simt.com.cn](mailto:liug@simt.com.cn); [Bachelor's degree information not provided]; Laboratory of Physical Biology, Shanghai Institute of Applied Physics, Chinese Academy of Science (Ph.D., 2009), Professor, Dr. Chunhai Fan, Biosensor research based on the conformational switch of the DNA nanostructures; Postdoctoral Researcher at SIMT (2009–2011), Dr. Jun Hu, Research of highly sensitive quantitative methods of DNA and related DNA certified reference materials; Senior Engineer at SIMT (2011–present), Metrological traceability research in bioanalysis.

I am interested in electrochemical biosensing research for highly sensitive miRNA analysis. We are constructing different 3-D probes that have great potential to improve the effect of spatial control and hybridization. I am also interested in metrological traceability research for nucleic acid quantification. We are paying attention to the research of quantitative methods that are traceable to SI units by comparing different bioanalysis methods, including HP-ICP-MS, UV, and digital PCR, estimating the uncertainty of the results and developing certified reference materials. I want a one-year exchange scholar position in a bioanalysis laboratory.

Abstract Title: *Highly sensitive miRNA analysis using stem-loop probes carried by...*

BIOL Division

**16. Ashish Garg;** Department of Chemistry, Brown University, 324 Brook St., Box H, Providence, RI, 02912; 401-345-2509, [ashish\\_garg@brown.edu](mailto:ashish_garg@brown.edu); Banaras Hindu University, India (M.S., Org Chem, 2001); Indian Institute of Technology Kanpur, India (Ph.D., 2009), Prof. Vinod K. Singh, Crafting of D-glucose in total synthesis of biologically active natural products; Postdoctoral Research Associate at Brown University (2009–present), Prof. David E. Cane, Mechanistic investigation in polyketide biosynthesis.

I am seeking a faculty position at a four-year college focused on undergraduate teaching and research. I have taught undergraduate lab sections in organic chemistry and instrumentation and have mentored undergraduate researchers. I thoroughly enjoy teaching and have experience as an instructor and a teaching assistant. My research will focus on small-molecule natural products of biological importance. The tools of organic synthesis and structure elucidation (i.e., NMR, MS) will be used to probe the chemical basis of these important biological phenomena.

Abstract Title: *Stereo specificity and mechanism of methyl group epimerization of the...*

BIOL, ORGN Divisions

**17. Jason Gavenonis;** Department of Chemistry, Tufts University, 62 Talbot Ave., Medford, MA 02155; [jason.gavenonis@tufts.edu](mailto:jason.gavenonis@tufts.edu); University of Pennsylvania (B.A., 2003); Boston College (Ph.D., 2010), Prof. Marc L. Snapper, Tandem reactions of dienes generated by enyne metathesis; NIH-IRACDA Postdoctoral Fellow at Tufts University (2010–present), Prof. Joshua A. Kritzer, Development of new peptide-based inhibitors of Hsp90.

I'm seeking a position at a liberal arts college or small university where research is valued as an essential component of undergraduate education. During my postdoctoral training, I had the opportunity to mentor a number of undergraduate researchers while teaching organic chemistry as an adjunct. My research will combine my graduate work in organometallic chemistry with my postdoctoral training in chemical biology to explore the organometallic chemistry of peptides and proteins. My educational interests include the modification of laboratory courses to incorporate research-based problems and the use of technology—both in and out of the classroom—to augment lecture-format courses.

Abstract Title: *Exploring alternate modes of Hsp90 inhibition with peptides*

ORGN, BIOL, INOR Divisions

**18. Terrence Neumann;** School of Pharmacy, Concordia University Wisconsin, 12800 North Lake Shore Drive, Mequon, WI 53097; [terrence.neumann@cuw.edu](mailto:terrence.neumann@cuw.edu); University of Wisconsin-River Falls, (B.S., 2005); University of Minnesota Duluth (M.S., 2011), Dr. Subhash Basak, Relative chirality index: A novel approach to the characterization of molecular chirality; Marquette University (Ph.D., 2013), Dr. Daniel Sem, NMR and computational characterization of protein structure, dynamics, and ligand binding.

My goal is to obtain a tenure-track faculty position at a primarily undergraduate university where teaching is the focus, yet student research is encouraged. I intend to convey my passion for the sciences to students by presenting engaging and timely material. By incorporating research projects into coursework, I will present concepts in a real-world environment and expose students to a different learning atmosphere. My research program will focus on using an interdisciplinary approach to find novel inhibitors for proteins in *Mycobacterium tuberculosis*. Students will be exposed to drug discovery techniques used in graduate school labs and the pharmaceutical industry.

Abstract Title: *Solution structures and models describing the thioredoxin system...*

BIOL, COMP Divisions

**19. Julie A. Pollock;** Department of Chemistry, University of Illinois at Urbana-Champaign, RAL 457 90-5, 600 S. Mathews, Urbana, IL 61801; [julie.pollock@gmail.com](mailto:julie.pollock@gmail.com); Hope College (B.S., 2006); Duke University (Ph.D., 2011), Dr. Dewey G. McCafferty, Examination of the role of lysine specific demethylase 1 (LSD1) and associated proteins in breast cancer proliferation using 2-phenylcyclopropylamine inhibitors; Postdoctoral Research Associate at University of Illinois at Urbana-Champaign (2012–present), Dr. John Katzenellenbogen, Synthesis of small molecule modulators of nuclear receptor function.

My research interests align at the interface of chemistry and biology, and in particular, I am interested in using small molecules to understand mechanisms of cancer development and progression. Students in my laboratory will employ organic synthesis, biochemistry, and cellular biology to answer these questions. I have had significant experience teaching undergraduates in organic chemistry and have developed and taught a freshman seminar course for nonmajors. My career goal is to teach and invest in students at a primarily undergraduate institution.

Abstract Title: *Modulation of nuclear receptor function at multiple levels: Agonist and...*

BIOL, ORGN Divisions

**20. Yftah Tal-Gan;** Department of Chemistry, University of Wisconsin–Madison, 1101 University Ave., Madison, WI 53706; [yftah.t@chem.wisc.edu](mailto:yftah.t@chem.wisc.edu); The Hebrew University of Jerusalem (B.S., 2001; M.S., 2006; Ph.D., 2011), Prof. Chaim Gilon (Chem) and Prof. Alexander Levitzki (Bio), Development of new peptide-based inhibitors of Protein Kinase B (PKB/Akt) as potential drugs for cancer; Postdoctoral Research Associate at University of Wisconsin–Madison (2011–present), Prof. Helen E. Blackwell, Development of peptide-based tools and materials to study quorum sensing in *Staphylococcus aureus*.

I seek a faculty position in chemistry at a Ph.D.-granting university. My interest in academic positions is multifaceted. First, I plan to develop an interdisciplinary research program incorporating organic chemistry, biochemistry, and molecular biology to focus on using cyclic peptides to study diverse biological systems and delineate signaling pathways' mechanisms within prokaryotic and eukaryotic cells. Second, I find teaching enjoyable and rewarding, with seven years' experience as TA in undergraduate classes (general and organic chemistry) and as lab instructor (organic and analytical chemistry). I eagerly anticipate teaching and mentoring students while simultaneously conducting high-quality research at the interface of chemistry and biology.

Abstract Title: *Cyclic peptides: Powerful chemical tools to elucidate biological pathways*

BIOL, ORGN, MEDI Divisions

**21. Aruna J. Weerasinghe**, Department of Chemistry, Duke University, Durham, NC, 27708; [aw181@duke.edu](mailto:aw181@duke.edu); University of Peradeniya, Sri Lanka (B.S., 2001; M.Phil., 2005); Western Michigan University (M.S., 2007; Ph.D., 2011), Dr. Ekkehard Sinn, Spectroscopic studies of new sensors for organophosphates, metals, and cyanide based on rhodamine and cholic acid derivatives; Postdoctoral Associate at Duke University (2011–present), Dr. Alvin Crumbliss, Ferric binding protein mediated iron transport in several Gram-negative bacterial strains.

I am seeking a faculty position at a primarily undergraduate institute where I can share my experience and interests with students. As a chemist with broad experience in chemistry (organic synthesis, inorganic synthesis, bioinorganic chemistry, and natural products chemistry), I am interested in continuing research in bacterial iron transport and fluorescent sensor development. Apart from research, I have combined two years of teaching experience as a Teaching Assistant at the undergraduate level. I am planning to build an externally funded research program for undergraduate students at an undergraduate research university.

Abstract Title: *Biophysical studies on the importance of the synergistic anion in iron...*

BIOL, INOR, ORGN Divisions

**22. Ji'En Wu;** Department of Chemistry, National University of Singapore, 3 Science Drive 3, S8-01-10, Singapore, S117543; +65 6516-4406, chmwujie@nus.edu.sg; Peking University (B.S., 1998); National University of Singapore (Ph.D., 2002), Dr. Leslie J. Harrison (Chem), Chemical studies on some Asian medical plants; Postdoctoral Researcher at Bristol University, School of Chemistry (2005–2007), Prof. Tom J. Simpson (FRS), Biosynthesis of mupirocin; Research Fellow at the Institute of Molecular and Cell Biology (Singapore), Prof. Lain-Hui Zhang, Small molecules that induce quorum sensing in microbes.

My research uses an interdisciplinary approach and techniques from analytical, synthetic, and biochemistry, and structural and molecular biology to understand how small molecules affect the life of microbes. I seek to find an academic position in a university and build a research program at the cutting edge of chemistry and biology, focusing on discovering small molecules' biological functions in microbes for developing next-generation antimicrobial drugs. I teach organic chemistry for final-year undergraduates and postgraduates (including writing and giving lectures) in the National University of Singapore. Additionally, I have assisted PIs in directing Ph.D. candidates in the United Kingdom and Singapore.

Abstract Title: *Applying NMR based metabolomic methods to study quorum sensing...*

BIOL, ORGN, MEDI, ANYL Divisions

**23. Mary E. (Mary Beth) Anzovino;** Department of Chemistry, University of Wisconsin–Madison, 1101 University Ave., Madison, WI 53706; anzovino@wisc.edu; Williams College (B.A., 2006), Prof. Sarah L. Goh, Exploring the synthesis of new polymeric materials; University of Wisconsin–Madison (Ph.D., anticipated December 2013), Prof. John W. Moore, Development of new research-inspired general chemistry laboratory experiments and a survey instrument to assess student awareness of and attitudes toward scientific research.

My ideal faculty position involves balancing teaching and research at a primarily undergraduate or master's-granting institution. My graduate research experience includes synthetic organic methodology and chemical education. I have mentored undergraduate and graduate students and have extensive experience as a teaching assistant (running lab and discussion sections) and a TA training assistant (providing guidance to new TAs). My experiences in the research lab, teaching lab, and classroom have driven me to study the teaching and learning of organic chemistry in the future. Organic chemistry typically elicits negative feelings in undergraduate students; I aim to change that perception via research-informed practices.

Abstract Title: *From the bench to the blackboard*

CHED Division

## 24.– Withdrawn

**25. Sukanta Dolai;** Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis, 402 N. Blackford Street, Indianapolis, IN 46202; [sdolai@iupui.edu](mailto:sdolai@iupui.edu); Presidency College, Kolkata, India (B.S., 2003); Indian Institute of Technology, Kharagpur, India (M.S., 2005); The City University of New York (M.S., 2007; Ph.D., 2010), Prof. Krishnaswami Raja, Synthesis of drug/dye incorporated copolymer–protein hybrids and novel curcumin derivatives for imaging and therapeutic applications; Postdoctoral Research Associate at College of Staten Island/CUNY (2010–2011), Prof. Krishnaswami Raja, Synthesis of curcumin incorporated water-soluble polymers and curcumin decorated bionanoparticle conjugates; Postdoctoral Research Associate at Indiana University-Purdue University Indianapolis (2011–present), Dr. Rajesh Sardar, Ultrasmall “magic-sized” metal-chalcogenide nanoclusters: Synthesis, investigation of nanocluster formation kinetics, and surface ligation effect on photo physical and electronic properties.

My research and teaching interests lie primarily in materials, organic and polymer chemistry, and interdisciplinary areas such as biomaterials and Nan science. My research focuses on the production of novel Nan composite materials based on conducting polymers and semiconductor nanoclusters of various functionalities with uniform size and core composition. I have taught and assisted in undergraduate-level general and organic chemistry courses and have an interest in core teaching methodologies that provide a student with a compact scientific foundation. I plan to develop interdisciplinary and laboratory courses involving theories and applications of modern instrumentation techniques and focusing on undergraduate and master’s degree students.

Abstract Title: *Next generation nanomaterial composites based on “magic sized”...*

COLL, PMSE, ANYL, INOR Divisions

**26. Joseph Jankolovits;** Department of Chemical and Biomolecular Engineering, University of California, Berkeley, 2151 Berkeley Way, Berkeley, CA 94704, [jankolovits@berkeley.edu](mailto:jankolovits@berkeley.edu); Grinnell College (B.A., Chem, 2007); University of Michigan, Ann Arbor (Ph.D., Inor Chem, 2012), Dr. Vincent L. Pecoraro, Anion recognition, self-assembly, and luminescence properties of lanthanide metallacrowns; Postdoctoral Research Scholar at the Department of Chemical and Biomolecular Engineering, University of California, Berkeley (2012–present), Dr. Alexander Katz, Synthesis and dispersion stability of grafted polysaccharide coatings on oxide particles.

I seek to mentor the next generation of scientists through a research program in inorganic and materials chemistry. I am interested in supramolecular strategies for assembling discrete substrates into functional molecules, and functional molecules into materials and devices. My research program will contribute to this area through the design, synthesis, and surface immobilization of coordination macrocycles and clusters to address areas of need in energy, catalysis, and luminescent devices. My qualifications for an academic faculty position include experience teaching and mentoring students, facilitating academic and industrial collaborations, and writing grant proposals.

Abstract Title: *Single-pot synthesis of uniform glucan multilayers on oxide particles*

COLL, INOR, PMSE, CELL Divisions

**27. Sarah L. Perry;** Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637; [perrys@uchicago.edu](mailto:perrys@uchicago.edu); University of Arizona, Tucson (B.S., Hon, Chem Eng, 2002; B.S. Chem, 2003; M.S. Chem Eng, 2005); University of Illinois at Urbana-Champaign (Ph.D., Chem Eng, 2010), Professor Paul J. A. Kenis, Microfluidic platforms for the characterization of *in meso* membrane protein crystallization; Postdoctoral Fellow at the University of Chicago and the University of California at Berkeley (2011–present), Professor Matthew Tirrell, Structure and self-assembly of biomimetic polyelectrolyte and coacervate systems.

My research uses self-assembly, molecular design, and microfluidic technologies to generate biologically relevant microenvironments for the study and application of biomacromolecules. Individually, microfluidics represents an enabling technology for the time-resolved analysis of enzyme structural dynamics, while control over molecular interactions in self-assembling polyelectrolyte systems can be used to examine the interplay between biomacromolecules and the intracellular environment. Together, these capabilities can be coupled to generate artificial organelle-like structures for use in applications ranging from biochemistry to bioenergetics, biocatalysis, and biomedicine. Furthermore, this work has tremendous pedagogical potential to inspire students to work at the intersection of chemistry, biology, and engineering.

Abstract Title: *Biomimetic and microfluidic approaches to biomolecular function...*

COLL, BIOL Divisions

**28. Alexey V. Akimov;** Department of Chemistry, University of Rochester, 120 Trustee Road, Hutchison Hall 430, Rochester, NY 14627; [alexvakimov@gmail.com](mailto:alexvakimov@gmail.com); M. V. Lomonosov Moscow State University (M.S, 2007); Rice University (M.A., 2009; Ph.D., 2011), Dr. Anatoly B. Kolomeisky, Theoretical studies of molecular machines; Postdoctoral Research Fellow at University of Rochester/Brookhaven National Laboratory (2012–present), Dr. Oleg V. Prezhdo (University of Rochester) and Dr. James T. Muckerman (Brookhaven National Laboratory), Nonadiabatic molecular dynamics in nanoscale materials, Theoretical studies of photocatalytic water splitting; <https://sites.google.com/site/alexeyvakimov/>.

I'm a postdoctoral scholar specializing in theoretical and computational chemistry. Specifically, I am interested in developing accurate and efficient computational techniques and models for quantum and molecular dynamics with the emphasis on the large-scale systems. Potential applications include photovoltaic and photocatalytic systems, biological objects, solid-state nanostructures, and functional nanomaterials, to mention a few. I am interested in a professorship at a Ph.D.-granting institution, where I plan to establish my research group. The work will involve students from diverse specialties and backgrounds. I also plan to establish a strong educational program for graduate and undergraduate students in chemical and physical disciplines.

Abstract Title: *Computational chemistry for nanotechnology, sustainable energy, and...*

COMP, PHYS, FUEL Divisions

**29. Joseph L. Baker;** Department of Chemistry, University of Chicago, 5735 S. Ellis Avenue, Chicago, IL 60637; [jlbaker@uchicago.edu](mailto:jlbaker@uchicago.edu); University of Nevada, Las Vegas (B.S., Physics, 2003); University of Arizona (Ph.D., Physics, 2011), Dr. Florence Tama (Chem and Biochem), Simulation studies of transmembrane proteins and bacterial pili; Postdoctoral Scholar at the University of Chicago (2012–present), Dr. Gregory Voth, computational studies of actin filaments and actin-binding proteins, and coarse-graining of large protein complexes; [vothgroup.uchicago.edu/group/voth-group-member/joe-baker](http://vothgroup.uchicago.edu/group/voth-group-member/joe-baker).

I am interested in large biomolecular systems and how computational methods and coarse-graining can be used as tools to understand their physical and biochemical properties. I would like to both teach and develop a research program in computational and theoretical chemistry that incorporates undergraduates at a four-year college. During my Ph.D., I had the opportunity to teach a lecture course that implemented interactive teaching methods and to administer an REU program that transitioned community college students to the university. This past summer, I was a research mentor for four undergraduates and two high school students at the University of Chicago.

Abstract Title: *Molecular dynamics simulations of large biomolecular complexes*

COMP Division

**30. Ryan G. Coleman;** Dept. of Pharmaceutical Chemistry, University of California, San Francisco, San Francisco, California 94158; 215-280-9645, [ryan.g.coleman@gmail.com](mailto:ryan.g.coleman@gmail.com); Marietta College (B.S./B.A., 2002.); Tufts University (M.S., 2004); University of Pennsylvania (Ph.D., 2009), Dr. Kim Sharp, Shortest geometric paths analysis in structural biology; NIH NRSA Postdoctoral Fellow [Year not provided], Dr. Brian Shoichet, Studying molecular docking.

I am seeking a faculty position at a doctorate-granting research institution, in a joint appointment between a biomedical or chemical department and a computer science department. I am prepared to teach students skills from the chemical to the computational. I am well suited to mentor students who wish to cross-train in both the experimental and computational fields, or students who wish to focus on one field and collaborate with others who can work on related problems. I plan to collaborate with other laboratories that have discovered interesting protein targets and pathways to develop new chemical tools and potential drugs.

Abstract Title: *Molecular recognition studied using computation and experiment*

COMP, BIOL Divisions

**31. Haining Liu;** Department of Chemical and Biological Engineering, University of Alabama, Tuscaloosa, AL 35487; hliu38@eng.ua.edu; Wuhan University, China (B.S., 2003); University of Windsor, Canada (Ph.D., 2009), Dr. James Gauld, Computational investigations into nucleic acid-related chemistry; Postdoctoral Researcher at the University of Mississippi (2009–2012), Dr. Robert Doerksen, Computational study on the origin of the toxicity of an antimalarial drug, primaquine, and computer-aided design of a novel ligand of the cannabinoid receptor; Postdoctoral Researcher at the University of Alabama (2012–present), Dr. C. Heath Turner, Computational study of the fundamental properties of imidazole-based CO<sub>2</sub> capture materials and the fundamental interactions during ligand-directed nanoparticle synthesis.

My research interest lies in applying computational chemistry methods to address some of the major concerns currently facing our society. Some examples include the design of new greenhouse gas capture materials and the elucidation of the reaction mechanisms involved in biofuel catalysis. I have experience in teaching lectures in a graduate course and supervising undergraduate students. In particular, one of the undergraduate students has been included as a coauthor of a published paper. I also have experience in assisting with proposal writing as a postdoctoral researcher at the University of Alabama. I seek a faculty position at a research university.

Abstract Title: *Computational investigations into the chemistry of biomolecules and...*

COMP, PHYS Divisions

**32. Peter Kekenes-Huskey;** 9500 Gilman Dr., M/C 0365, La Jolla, CA 92093-0365; pkekeneshuskey@ucsd.edu; University of North Carolina at Asheville (B.S., Chem, 2001); California Institute of Technology (Ph.D., Chem, 2009), Dr. William A. Goddard, III, A Monte Carlo-based torsion construction algorithm for ligand design; Postdoctoral Scholar at University of California, San Diego (2010–present), James A McCammon, Multiscale simulation of cardiac disease; <http://mccammon.ucsd.edu/~huskeypm/>.

As an aspiring academic researcher at a research institution, I seek insight into the cellular bases of disease that elude experimental protocols. What excites me about this work is leveraging biophysics to advance basic research and ultimately improve quality of life. Vital to this research is my expertise in physical chemistry, algorithm design, software engineering, and applied math. I am enthusiastic about sharing my passion for science with students and colleagues and instilling the interdisciplinary perspective that my mentors cultivated in me. The academic environment provides the perfect interface for conducting cutting-edge science while shaping the newest generation of scientists.

Abstract Title: *Multiscale modeling of calcium signaling in cardiac muscle: An...*

PHYS Divisions

**33. Sunghwan Kim;** National Center for Biotechnology Information (NCBI), National Library of Medicine (NLM), National Institutes of Health (NIH), 8600 Rockville Pike, Bldg. 38A, Rm. 8N811k, Bethesda, Maryland, 20894; [kimsungh@ncbi.nlm.nih.gov](mailto:kimsungh@ncbi.nlm.nih.gov); Hanyang University (B.S., 1999; M.S., 2011); University of Georgia at Athens (Ph.D., 2007), Prof. Henry F. Schaefer, Applications of density functional theory for studying radiation-induced DNA damage; Postdoctoral Visiting Fellow (2007–2011) and Research Fellow (2011–present) at NCBI NLM NIH, Dr. Stephen H. Bryant, Development of public chemical biology information resources for biological assay data analysis and drug discovery.

I am seeking a tenure-track faculty position at a Ph.D.-granting institution, where I will build an interdisciplinary research program in translational science. I have extensive research experience (with 31 peer-reviewed publications) in diverse scientific areas, covering inorganic and physical chemistry, cheminformatics, and computer science. I also have teaching and mentoring experience at both the undergraduate and graduate level. My research program will focus on (i) developing informatics tools for drug discovery and applying them for drug repurposing to treat rare and neglected diseases, and (ii) developing prediction models for phototoxicity and photosensitivity of drug molecules.

Abstract Title: *PubChem and PubChem3D: Public chemical information resources for...*

COMP, PHYS, MEDI, BIOL Divisions

**34. Alex Kutana;** Mechanical Engineering and Materials Science, Rice University, 6100 Main St., Houston, TX 77005; [kutana@rice.edu](mailto:kutana@rice.edu); Kiev National T. Shevchenko University (B.S., 1996); University of Houston (Ph.D., 2003), Dr. J. W. Rabalais (Chem), Structure and gas adsorption kinetics for monocrystalline surfaces studied with low-energy ion scattering; Postdoctoral Researcher at California Institute of Technology (2003–2008), Dr. Giapis, Computational nanoscience; Postdoctoral Researcher at Rice University (2012–present), Dr. Yakobson, Computational chemistry and materials science, computational nanoscience; <http://alexkutana.net/>.

My research focuses on theoretical and computational studies of electronic, chemical, and mechanical properties of molecules and condensed phase systems, with the aim of advancing our understanding of the nanoscale world. My most recent research effort concentrates on 2-D systems. My goal is to establish a high-impact, internationally recognized program in computational chemistry and the nanosciences. I want to teach and direct the research of undergraduate and graduate students at a Ph.D.-granting university.

Abstract Title: *Dynamics of hot electron relaxations*

COMP, PHYS Divisions

**35. Sara E. Nichols;** Department of Pharmacology, 9500 Gilman Drive M/C #0365, University of California, San Diego, La Jolla CA, 92093-0365; 858-822-1469, [senichols@ucsd.edu](mailto:senichols@ucsd.edu); New York University (B.A., 2003); Yale University (M.S., 2006; Ph.D., 2009), Prof. William L. Jorgensen, High-throughput methods for computer-aided drug design pertaining to flexibility, selectivity and lipophilicity; Postdoctoral Researcher at University of California, San Diego, (2009–present), Prof. J. Andrew McCammon, Evaluation and use of molecular dynamics methods for virtual screening, docking and classification; <http://mccammon.ucsd.edu/~snichols>.

My work focuses on designing and using computational techniques for investigating allostery of therapeutically relevant proteins. I've studied and applied computational methods—including informatics-based techniques and complementary physics-based molecular modeling—to a variety of different host, guest, and delivery proteins, such as reverse transcriptase, dihydrofolatereductase, cyclotides, and cucurbiturils, G-proteins and G-protein coupled receptors, and nuclear receptors. In pursuing the structure–function–activity relationships of signaling biomolecules, I hope to carry out mentorship-focused research in a pharmacology-oriented academic setting.

COMP, BIOL, MEDI Divisions

Abstract Title: *Allostric regulation of protein motion and function*

**36. Patric Schyman**

Abstract Title: *Computer aided chemistry for understanding DNA damage, catalysis,...*

**37. Daniel J. Sindhikara;** Department of Science and Engineering, Ritsumeikan University, 1-1-1 Noji-Higashi, Kusatsu, Shiga 525-8577, Japan; [sindhikara@gmail.com](mailto:sindhikara@gmail.com); Richard Stockton College of New Jersey (B.S., 2004); University of Florida (M.S., 2005; Ph.D., 2009), Dr. Adrian E. Roitberg, A sampling of molecular dynamics; Postdoctoral Fellow at Nagoya University (2009–2010), Dr. Yuko Okamoto, Design of enhanced sampling methods; Postdoctoral Fellow at the Institute for Molecular Science/Ritsumeikan University (2010–present), Dr. Fumio Hirata, Development of 3-D–RISM theory towards drug design; [www.dansindhikara.com](http://www.dansindhikara.com).

I am interested in computational chemistry using advanced solvation and enhanced sampling techniques toward biomolecular study, particularly drug design. I hope to interest students from multiple fields including chemistry, biochemistry, physics, and computational science. I was a TA for several years and also led a lecture class in algebra-based physics, earning both departmental and university teaching awards. I want to teach and direct the research of graduate or eager undergraduate students, or both, at either a four-year college or a university.

Abstract Title: *Equilibrium solvation site analysis without simulation*

COMP, PHYS, BIOL, MEDI Divisions

**38. Eduardo M. Sproviero;** Department of Chemistry & Biochemistry, University of the Sciences, 600 S. 43rd St., Philadelphia, PA 19104; 267-295-3189, [e.sproviero@usciences.edu](mailto:e.sproviero@usciences.edu); University of Buenos Aires (M.S., 1994; Ph.D., 2003), Dr. Gerardo Burton (Chem) and Dr. Ruben H. Contreras (Phys), Study of conformational and structural effects in molecules, development of methods based on orbital interactions to analyze their electronic mechanisms; Postdoctoral Fellow at Yale University Department of Chemistry (2004–2010); Dr. Victor S. Batista, QM/MM models and water splitting mechanism of the O<sub>2</sub>-evolving complex in photosystem II and inorganic complexes, QM/MM characterization of functionalized TiO<sub>2</sub> surfaces as photocatalytic devices for oxidation chemistry, EXAFS spectroscopy as a tool to determine molecular structures of transition metal-containing species (e.g., active sites in proteins and inorganic complexes), electronic structure analysis based on QM/MM and NMR methodologies applied to the retinyl chromophore in rhodopsin; Postdoctoral Fellow at the University of the Sciences, Department of Chemistry & Biochemistry (2011–2013), Dr. Vojislava Pophristic, Development of a methodology that decomposes and quantifies intramolecular interactions, including electrostatic interactions, charge delocalization pathways, and core repulsions, development of a methodology for determining oligomer structures without using fitted parameters, which uses QM at short distances and effective fragment potentials (EFP) at longer distances to model nonbonded interactions; [www.qo.fcen.uba.ar/Grupos/burtongrp-en.htm](http://www.qo.fcen.uba.ar/Grupos/burtongrp-en.htm), [www.chem.yale.edu/~batista/](http://www.chem.yale.edu/~batista/), [www.gradschool.usciences.edu/faculty/pophristic-vojislava](http://gradschool.usciences.edu/faculty/pophristic-vojislava).

My plan is to use information extracted from biological systems in developing “bio-inspired” technologies. Projects include the designing and elucidating mechanisms of foldamers combined with inorganic metallo complexes, as synthetic second coordination spheres for biologically inspired catalysts. I’m also interested in developing formal methods allowing decomposition of covalent and non-covalent interactions to aid in understanding the forces governing molecular interactions. I taught several courses during my Ph.D. and codirected many students during my postdoctoral training. I’d like to motivate students and postdocs to form a research group, and I want to teach in schools that offer undergraduate or undergraduate/graduate degrees.

Abstract Title: *Development and application of computational methods to biological...*

COMP, PHYS, ENFL, CATL Divisions

**39. Robert V. Swift;** Department of Chemistry and Biochemistry, University of California, San Diego, 9500 Gilman Dr., Urey Hall 3213, La Jolla CA 92093-0340; 858-534-9617, [rvswift@ucsd.edu](mailto:rvswift@ucsd.edu); University of California, Santa Barbara (B.S., *Highest Honors*, 2005); University of California, San Diego (M.S., 2007); University of California, San Diego (Ph.D., 2009), Dr. Andrew J. McCammon, Structure–function relationships in enzymes of the nucleotidyltransferase superfamily: RNA ligation and mRNA capping; Postdoctoral Researcher at the University of California, San Diego (2009–present), Dr. Rommie E. Amaro, Computational drug discovery and optimization, Computational and theoretical characterization of enzyme catalysis.

I am interested in a position at a research-intensive, primarily undergraduate institution. My research interests focus on developing and applying physics-based computational methods to discover and optimize small molecule modulators of biomolecular function (e.g., enzyme inhibitors). In addition to mentoring undergraduate researchers, I'm interested in integrating peer-led team learning approaches into my teaching. I have extensive teaching and mentoring experience and am currently an instructor of record for Chem 13, The Chemistry of Life, at UCSD.

Abstract Title: *Physics-based, computational approaches to ligand discovery and design*  
BIOL, PHYS Divisions

**40. Swapnil Liladhar Fegade;** Department of Chemical Engineering, University of North Dakota, 3702 Berkeley Drive, Apt # 5, Grand Forks, ND 58203; Cell phone: 701-215-0371, [swapnil.fegade@my.und.edu](mailto:swapnil.fegade@my.und.edu), [swapnil.und@gmail.com](mailto:swapnil.und@gmail.com); University of Mumbai, Institute of Chemical Technology (formerly UDCT, currently known as ICT-UICT-Mumbai), India (B.Tech., 2005); University of North Dakota (Ph.D., Chem Eng, anticipated 2013), Dr. Brian Tande, Catalytic conversion of cracked crop oil to produce aromatic compounds.

I am a chemical engineer with industrial managerial experience in polymer processing, and I am currently pursuing my Ph.D. in chemical engineering with a focus on renewable energy research. My current research interests include process development and optimization, design of experiments (DOE), renewable feedstocks for biofuels and chemical production, aromatization, catalysis, zeolites, petroleum refining processes such as thermal cracking and catalytic cracking and reforming, polymer science, and engineering. As a graduate student I have seven semesters of teaching experience. I mentored the undergraduate research of two students. I am an active student volunteer at Altru Health System.

Abstract Title: *Catalytic processes for the production of biobased chemicals and...*  
ENFL, FUEL Divisions

## 41 Gabriel LeBlanc

Abstract Title: *Solar energy conversion using biohybrid electrodes based on...*

**42. Kumudu Mudiyanselage;** Chemistry Department, Building 555, Brookhaven National Laboratory, P.O. Box 5000, Upton, NY 11973; 631-344-4347, [kmudi@bnl.gov](mailto:kmudi@bnl.gov), [mudiyanselagek@yahoo.com](mailto:mudiyanselagek@yahoo.com); University of Colombo, Sri Lanka (B.S., 1999); University of Illinois at Chicago (PhD, 2008), Prof. Michael Trenary, Hydrogenation and dehydrogenation of nitrogen containing species on the Pt(111) surface; Research Associate at Pacific Northwest National Laboratory (2008–2011), Dr. Janos Szanyi, Investigation of  $\text{NO}_x$  storage and reduction reactions on model automotive catalysts; Research Associate at Brookhaven National Laboratory (2011–present), Dr. Dario Stacchiola, Investigation of catalytic reactions on copper-based model systems; <http://www.bnl.gov/chemistry/bio/MudiyanselageKumudu.asp>.

Teaching and interacting with students has always been a fundamental facet of my career, and I am interested in continuing that as a part of my professional life. An underlying theme of my current research has been the fundamental research approach for the atomic-scale understanding of catalytic reactions using surface science tools. I am interested in continuing to pursue this goal by extending the research to practical powder catalysts. I would like to focus on both teaching and research, and I am seeking a tenure-track faculty position at either a Ph.D./M.S.-granting university or a four-year undergraduate college.

Abstract Title: *Importance of the metal–oxide interface in catalysis: In situ studies...*

ENFL, COLL, PHYS Divisions

**43. Christopher James Patridge;** Naval Research Laboratory, 4555 Overlook Ave. SW, Washington, DC 20375; phone: 202-404-3749, cell phone: 315-529-0501, [christopher.patridge.ctr@nrl.navy.mil](mailto:christopher.patridge.ctr@nrl.navy.mil); University at Buffalo, The State University of New York (B.A., Chem, 2002; Ph.D., Chem/Mat, 2011), Prof. Sarbajit Banerjee, Prof. Esther S. Takeuchi, Chemically and temperature induced phase transformations of metal vanadates; NRC Postdoctoral Research Associate at the Naval Research Laboratory (2011–present), Dr. Karen Swider-Lyons, Fundamental studies of Li-ion cells to understand the solid electrolyte interphase using XAS, EIS, and electrochemical methods.

I am interested in fundamental studies and the development of novel nanoscale intercalation compounds for both Li-ion and Na-ion electrochemical cells through materials synthesis methods and electrochemical characterization, as well as accessing cutting-edge research facilities through general-user research proposals. I have experience teaching laboratories in several core chemistry disciplines and would be interested in teaching at the undergraduate and graduate level, or both, in core chemistries and in specific areas such as spectroscopy, materials, and instrumentation. I will foster students and give them a solid foundation for their present and future academic success.

Abstract Title: *Detailed Raman and X-ray analysis of electrolyte dopants in Li-ion...*

PHYS, ENFL Divisions

**44. Clara P. Adams;** Department of Chemistry, Western Michigan University, 3425 Wood Hall, Kalamazoo, MI 49008; [clara.p.adams@wmich.edu](mailto:clara.p.adams@wmich.edu); University of North Carolina at Charlotte (B.A., Chem, 2007); Western Michigan University (Ph.D., Chem, 2013), Dr. Sherine O. Obare, Synthesis and characterization of nanoscale materials for biosensor development.

My goals are to obtain a postdoctoral position, followed by a faculty position, at a four-year university. My research training involves materials science, environmental chemistry, and nanotechnology. I've designed sustainable synthetic pathways to produce various metallic nanoparticles for fabricating chemical/bio-sensors. I've taught general chemistry laboratory courses, developed an inquiry-based integrated biological chemistry lab unit, and mentored undergraduate and high school students in research. I aspire to teach at an institution where I can impart strong knowledge of fundamental and advanced scientific concepts within chemistry while developing a nationally recognized research program in sustainable nanoscale science.

Abstract Title: *Shape-controlled nanoscale materials and their applications as...*

ENVR Division

**45. Robert F. Hansen;** Department of Chemistry, Indiana University Bloomington, 800 E. Kirkwood Avenue, Bloomington, IN 47405; [rjhansen@indiana.edu](mailto:rjhansen@indiana.edu); Baldwin Wallace University (formerly Baldwin-Wallace College, B.S., 2006); Indiana University (Ph.D., anticipated Dec 2013), Dr. Philip Stevens, Development and deployment of instrumentation for measurement of total hydroxyl radical reactivity.

I seek a faculty position at a primarily undergraduate institution or a postdoctoral research position with a strong teaching component. My graduate research has focused on the development and field deployment of instrumentation to measure the reactivity of hydroxyl radical in the atmosphere and has led me to some unique opportunities. I also have experience as a teaching assistant for undergraduate lab courses and am participating in developing a laboratory investigation for an undergraduate physical chemistry course. In my teaching, I intend to guide students to a deep understanding of chemistry and its relevance to everyday life.

Abstract Title: *Investigation of hydroxyl radical reactivity in a suburban environment*

ENVR, ANYL Divisions

**46. David T. R. Stewart;** Department of Chemistry, University at Buffalo, 612 Natural Sciences, Buffalo, NY 14260; 716-696-0382, [dts8@buffalo.edu](mailto:dts8@buffalo.edu); Binghamton University (B.S., Biochem, 2005); University at Buffalo, The State University of New York (Ph.D., Chem, anticipated 2014), Dr. Diana S. Aga, Assessing the effects of earthworm exposure to quantum dot nanoparticles; [http://www.acsu.buffalo.edu/~dianaaga/Grad\\_Stu.html](http://www.acsu.buffalo.edu/~dianaaga/Grad_Stu.html).

I am seeking a position at an institution of higher learning that places a strong emphasis on undergraduate education and that values research and publication as an important learning tool at all levels. I have a strong background in education and was awarded an honorable mention for excellence in graduate student teaching. My research will focus on using liquid chromatography tandem mass spectrometry (LC-MS/MS) to study the biochemical effects of environmental contamination. LC-MS/MS is a powerful technique increasingly being used in academic and industrial research, but it is not yet widely taught at the undergraduate level.

Abstract Title: *Assessing the effects of quantum dots in the terrestrial environment...*

ANYL, ENVR, CHED Divisions

**47. Jennifer S. Atchison;** Energy Materials Group, INM-Leibniz Institute for New Materials, Campus D2 2, 66123 Saarbrücken, Germany; [Jennifer.Atchison@INM-Gmbh.de](mailto:Jennifer.Atchison@INM-Gmbh.de); Drexel University, Philadelphia, PA (B.S., 2000); American Competitiveness Institute, Philadelphia PA (1999–2000); JDS Uniphase, Ewing, NJ (2000–2002), Limited Brands, Springfield PA (2002–2004); Drexel University (PhD., 2012), Dr. Caroline Schauer, Electrospinning fluorescent hybrid polyelectrolyte ultrafine fibers; Senior Materials Chemist at Energy Materials Group, INM-Leibniz Institute for New Materials (2012–present), Dr. Volker Presser, Electrospinning polymer derived ceramics-carbide derived carbon ultrafine fibrous mats as binderless electrodes for supercapacitors.

Ideally, I would like to join a dynamic materials science or multidisciplinary department that is looking for a candidate with a strong background in photonics, organic chemistry, and materials. I would prefer a tenure-track position at a research university but would also consider a position at a college with a strong tradition of undergraduate research. My research interests include exploiting nanofiber properties for improved electrode design for energy harvesting and storage, nanofiber sensors, and designing multifunctional scaffolds for cell culturing. In addition to my technical research, I am interested in continuing my work in STEM education.

Abstract Title: *Interactions at boundaries: Exploring surface area, length scales, and...*

FUEL, POLY Divisions

**48 Liwei Zhang**

Abstract Title: *Development of a 2D reactive transport model to predict acid gas...*

**49 – Tianbiao Liu**

Abstract Title: *Half-sandwich Fe electrocatalysts for H<sub>2</sub> oxidation and production*

**50. Pius O. Adelani;** Center for Material Science of Actinides, Energy Frontier Research Center, University of Notre Dame, Notre Dame, Indiana 46556; padelani@nd.edu; University of Ibadan, Nigeria (B.S., 2000; M.S., 2003); University of Notre Dame (Ph.D., 2011), Prof. Thomas E. Albrecht-Schmitt, Syntheses, structure elucidation, and properties of novel actinide diphosphonates and carboxyphosphonates; Postdoctoral Researcher at the University of Notre Dame (2012–present), Prof. Peter C. Burns, Exploratory synthesis and X-ray characterization of uranyl compounds: Uranyl peroxide clusters and actinide–organic hybrid materials.

I am pursuing a tenure-track faculty position at an R1/M.S.-granting institution, where I plan to manage an active research group and mentor future scientists. I seek to teach general and inorganic chemistry at any level and organic chemistry to undergraduates. My research background will provide opportunities for individuals who are interested in X-ray crystallography and spectroscopic techniques. My research interest focuses on the design and synthesis of inorganic materials, hybrid materials, and clusters to address challenges of renewable energy; the ideal is to develop methods for controlling the formation of the structures as a means of tailoring their physical properties.

Abstract Title: *Correlations and differences between uranium(VI) arsonates and...*

INOR Division

**51. Liyana A. Wajira Ariyadasa;** Department of Chemistry, Western Michigan University, 1903 W. Michigan Ave., Kalamazoo, MI 49008; [wajira.ariyadasa@wmich.edu](mailto:wajira.ariyadasa@wmich.edu); University of Peradeniya, Sri Lanka (B.S., Chem, 2002; M.S., Env Sci, 2006); Western Michigan University (Ph.D., anticipated 2013), Prof. Sherine Obare, Well-defined metal nanoparticles as electron and energy storage materials.

My work has focused on developing sustainable procedures for developing well-defined nanoscale materials and understanding their physical and chemical properties. My research has shown unique energy storage properties of nanomaterials with controlled size. I have three years of teaching experience both in a classroom and in training undergraduate and high school students in research. My teaching has led to developing problem-based laboratories, and I aim to establish a research and educational program to train undergraduate and graduate students in nanoscale science. I am interested in improving pedagogy at the undergraduate and graduate level and ensuring the promotion of interdisciplinary science.

Abstract Title: *Metallic nanoparticles for biorenewables conversion via hydrogenation...*

INOR, PHYS, ENFL, COLL Divisions

**52. Andrew D. Basner;** Department of Chemistry, Syracuse University, 1-014 Center for Science and Technology, Syracuse, NY 13244; 317-908-3045, [adbaser@syr.edu](mailto:adbaser@syr.edu); Indiana University-Purdue University Indianapolis (IUPUI) (B.S., 2008); Syracuse University (Ph.D., anticipated December 2013), Dr. Sponsler, Synthesis and characterization of tri-ruthenium complexes for use as electron reservoirs in dye-sensitized solar cells; [www.adbasner.com](http://www.adbasner.com).

I am interested in synthesizing and characterizing new compounds in order to develop novel ways to capture solar energy. I am also interested in chemical entrepreneurship and commercializing research with applicability to and impact on the commercial world. I have been an assistant for a large number of general and organic chemistry courses over an eight-year period in addition to mentoring numerous undergraduate and REU students. I want to teach and mentor students at either a four-year college or a master's degree-granting institution.

Abstract Title: *Synthesis and characterization of polyruthenium dyes for solar cells and...*

INOR, ORGN, SCHB Divisions

**53. Jakoah Brgoch;** Materials Research Laboratory, Room 2027B, University of California, Santa Barbara, CA 93106; 309-531-7907, [jrbrgoch@mrl.ucsb.edu](mailto:jrbrgoch@mrl.ucsb.edu); Illinois State University, (B.S., Chem, 2006); Iowa State University, (Ph.D., Chem, 2012), Prof. Gordon J. Miller, Controlling magnetic structure in extended solids using targeted chemical compositions; Postdoctoral Research Associate at University of California, Santa Barbara (2012–present), Prof. Ram Seshadri, Phosphors for solid-state white lighting applications.

Combining expertise from my Ph.D. and postdoctoral work, I will establish a diverse and dynamic research group at a research-intensive university. By integrating my comprehensive background in experimental and computational solid-state chemistry, I will investigate the complex structures, compositions, and property relationships that exist in materials chemistry today, with a primary focus on discovering novel super-hard materials and complex magnetic ordering in metallic systems. Through this approach, I will teach students the framework of both theoretical and experimental techniques, cultivating a culture of interdisciplinary research from which the most complex problems can be explored and solved.

Abstract Title: *Materials design by first-principles*

INOR Division

**54 Thomas G. Gardner**

Abstract Title: *Functional supramolecular constructs of edge-binding, low-symmetry...*

**55. Sarina J. Dorazio;** Department of Chemistry, University at Buffalo, Amherst, NY 14260; sdorazio@buffalo.edu; Genesee Community College (A.S., 2000; A.A., 2007; A.S., 2007); University at Buffalo, State University of New York (B.A., 2008; Ph.D. 2013), Dr. Janet R. Morrow, Transition metal ion paraCEST contrast agents for MRI; <http://www.linkedin.com/pub/sarina-dorazio/45/54a/59b/>.

I'm seeking a tenure-track research faculty position upon completion of a postdoctoral appointment. My work has led to five publications (including two *JACS*), a book chapter, and a pending patent. Two additional publications are in preparation. I received the WCC-Eli Lilly and ACS-DIC travel awards. I am actively involved in science outreach at the middle school level and have integrated undergraduates into the research laboratory. I intend to be involved in science education and to encourage underprivileged students to pursue science. My independent research focus will incorporate bioinorganic chemistry, inorganic synthesis, and spectroscopic characterizations toward the design of contrast agents.

Abstract Title: *Transition metal ion complexes as MRI paraCEST contrast agents*

INOR Division

**56. Jeremiah J. Scepaniak;** Department of Chemistry, University of Washington, Campus Box 351700, Seattle, WA 98195-1700; 575-805-0829 *h index* = 6, [jjscapan@u.washington.edu](mailto:jjscapan@u.washington.edu); St. John's University (B.A., 2005), Prof. Brian Johnson, Model complex for the sulfide bridged Cu<sub>2</sub> cluster of *P. Stutzeri*; New Mexico State University (Ph.D., 2011), Prof. Jeremy M. Smith, High valent terminal iron nitrides; Postdoctoral Research Associate at University of California, Santa Barbara (2011–2012), Prof. Trevor W. Hayton, Tris-ketimine complexes of copper, Alcohol oxidation by Lewis acid assisted piperidine-n-oxide, and Efforts towards a uranium alkylidene; Postdoctoral Research Associate at the University of Washington (2012–present), Prof. D. Michael Heinekey, C–H bond activation by electrophilic Ir(III) cations; <http://www.linkedin.com/pub/jeremiah-scepaniak/45/9a0/29a>.

I am seeking a faculty position at a Ph.D.-granting institution that equally values research and teaching. My previous research has contributed to 10 publications so far, including 3 *JACS*, 2 *Angewandte Chemie*, and 1 *Science* article. I wish to recruit undergraduates—particularly those from underprivileged backgrounds—to conduct research, preparing them for graduate-level studies in STEM fields. My research groups' interests will be based in synthetic inorganic chemistry and will incorporate aspects of organometallic, polymer, and bioinorganic chemistry. For an in-depth description of my interests, please visit <http://www.linkedin.com/pub/jeremiah-scepaniak/45/9a0/29a>.

Abstract Title: *C–H bond activation by iridium (III) complexes supported by NHC...*

INOR Division

**57. Juliet Hahn;** Assistant Professor, Department of Chemistry, Francis Marion University, Florence, SC 29502; 803-955-6008, JHahn@fmarion.edu; University of South Carolina–Columbia (B.S., Magna Cum Laude, Phi Beta Kappa, Chem, [Year not provided]); State University of New York–Stony Brook (Ph.D., Org Chem, [Year not provided]), Prof. William leNoble, Stereoselectivity in heterocyclic amine; Postdoctoral Researcher at (1) Columbia University (organometallic [Year not provided]), Prof. Gerard Parkin, Transition metal organometallic pyrazoylborates, Cp metallocenes, and salen complexes of interest as metalloenzyme models and polymerization catalysts; (2) University of Wisconsin–Madison (org [Year not provided]), Prof. Richard Hsung, Synthetic organic chemistry—heterocyclic amine and pyrone synthesis, enamides and nonnatural amino acid chiral auxiliary of natural products of potential pharmaceutical interest; <http://JulietHahn.com>.

Excellent educator and PI researcher: documentation of excellent college-level teaching (see teaching evaluations on website) and increasing enrollment. Teaching: General, and organic chemistry lecture and lab, organometallics, bioorganic, organic spectroscopy, advanced organic (class size, 15–300, 95% white, 85% African American, 30% Hispanic) economically disadvantaged, honors students. Research as PI continuing from former faculty position (a) Carbon nanotube—materials, solar energy, (b) Photodimerization of DNA—Experimentally bio-organically model skin cancer, (c) Stereoselective synthetic methodology—Potential pharmaceuticals for Alzheimer's, (d) Teaching large lectures with increased retention opening STEM areas to students not naturally gifted in the sciences. Preferred institution: Primarily undergraduate college.

Abstract Title: *Carbon nanotube functionalization to develop electrically conductive...*

INOR, ORGN, BIOL Divisions

**58. Khadine A. Higgins;** Department of Chemistry, Indiana University Bloomington, Simon Hall 320 A, 212 S. Hawthorne Dr., Bloomington, IN 47405; [khhiggin@indiana.edu](mailto:khhiggin@indiana.edu); Lawrence University (B.A., 2004); University of Massachusetts, Amherst (Ph.D., 2012), Prof. Michael J. Maroney, Metal selectivity in the *E. coli* Ni(II)- and Co(II)-responsive transcriptional regulator, RcnR; Postdoctoral Fellow at Indiana University Bloomington (2012–present), Prof. David P. Giedroc, Structural studies of the multidomain protein, CstA.

I am seeking a faculty position at a primarily undergraduate institution. I attended a reputable liberal arts college, and as a result I know first-hand the value of a good undergraduate education. My research is at the interface of chemistry and biology, using both spectroscopic and biochemical techniques aimed at understanding metal selectivity and response in transcriptional metalloregulators as well as sulfur metabolism in *Staphylococcus aureus*. As a graduate student, I taught both general and inorganic chemistry labs. I have mentored both graduate and undergraduate students doing research in my lab.

Abstract Title: *Importance of Ni(II) to E. coli and sulfur to S. aureus*

INOR, BIOL Divisions

**59. Stefan M. Kilyanek;** Department of Chemistry, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA 02139; [smkilyanek@gmail.com](mailto:smkilyanek@gmail.com); Grand Valley State University (B.S., 2003); the University of Chicago (Ph.D., 2009), Prof. Richard F. Jordan, Mechanistic and computational studies of reactions relevant to olefin polymerization; Postdoctoral Associate at Massachusetts Institute of Technology (2010–present), Prof. Richard R. Schrock, Mechanistic studies of stereo-regular ring opening metathesis polymerization and fundamental studies of di-substituted alkylidene species.

I am pursuing a tenure-track position at a Ph.D.- or M.S.-granting institution. My research will focus on designing and synthesizing multimetallic systems for catalytic activation and conversion of small molecules, such as N<sub>2</sub> and CO<sub>2</sub>, to other chemical feedstocks. My students will learn organometallic synthesis and various physical inorganic methods, including mechanistic analysis, kinetics, computational modeling (MM/MD, DFT), and varied spectroscopic techniques. I enjoy teaching through research and have mentored several undergraduate students who wrote honors theses on their research. Through my teaching, I hope to excite students about the fundamental role of chemistry in all aspects of life.

Abstract Title: *Fundamental studies of the rearrangement and isomerization of...*

INOR, CATL Divisions

**60. Samuel E. Lohse;** University of Illinois at Urbana-Champaign, Department of Chemistry, 600 S. Mathews Ave., Urbana IL, 61801; 217-333-339, [slohse@illinois.edu](mailto:slohse@illinois.edu)); Idaho State University (B.S., Biochem, 2003; B.S., Chem, 2005; M.S., Chem, 2005); University of Oregon (Ph.D., Chem, 2011), Prof. Jim Hutchison, Direct synthesis of thiolate-protected gold nanoparticles using Bunte salts as ligand precursors: Investigations of ligand shell formation and core growth; Postdoctoral Researcher at the University of Illinois at Urbana-Champaign (2011–present), Prof. Catherine J. Murphy, Developing functionalized nanoparticles with predictably controlled bio fate and transport; <http://www.scs.illinois.edu/murphy/people/index.shtml>, <http://sustainable-nano.com/meet-the-scientists/#samlohse>.

My future research plans focus on investigating the fundamental chemistry of the growth mechanisms of functionalized nanoparticles and their transformations following exposure to biological or ecological systems. This research program is inherently interdisciplinary, and would benefit from the participation of students with interests in many different chemical fields (particularly inorganic, analytical, and biochemistry). I would like to establish a research program at a primarily undergraduate institution. Ultimately, I want to combine innovative education and research approaches to develop a comprehensive educational experience for undergraduate and master's-level chemistry students that provides them the opportunity to explore cutting-edge chemistry topics and research.

Abstract Title: *Biological interactions of gold nanoparticles (AuNPs): Understanding...*

INOR, COLL, BIOL Divisions

**61. Anusree Mukherjee;** Argonne National Laboratory, [Address not provided]; [Mukherjee@anl.gov](mailto:Mukherjee@anl.gov); University of Calcutta (B.S., 2003); Indian Institute of Technology, Bombay (M.S., 2005); University of Minnesota (Ph.D., 2011), Prof. Lawrence Que, Jr., Modelling iron-enzyme by synthetic complexes and testing their scope and reactivity toward hydrocarbon oxidation; Postdoctoral Research Associate at Argonne National Laboratory [Dates not provided], Dr. Karen L. Mulfort, Preparing different heterometallic supramolecular manifold for light-driven hydrogen production.

In my individual career, I want to teach and develop a research program that will give the students the opportunity to participate in energy-related research. Based on my educational background and my own experience, I will be glad to be part of a small college or university environment. I intend to motivate students in chemistry and encourage them to pursue higher studies.

Abstract Title: *Ultrafast charge separation in a cobaloxime photocatalyst...*

INOR, PHYS, BIOL Divisions

**62. Venkata S. Pavan K. Neti;** University of Texas at El Paso, El Paso, TX 79968; 864-643-8741, [vpneti@miners.utep.edu](mailto:vpneti@miners.utep.edu); Andhra University (B.S., 2004); Sri Venkateswara University (M.S., 2006); Clemson University and University of Texas at El Paso (Ph.D., 2009–present), Prof. Luis Echegoyen, Porous organic framework materials and novel fullerenes for organic photovoltaics.

I seek a faculty position at a teaching/research-intensive, primarily undergraduate institution. I plan to develop an interdisciplinary research program focusing on novel donor–acceptor organic based materials for photovoltaics and other applications. Additionally, I am eager to use my experience mentoring undergraduates in both the classroom and the laboratory. I am interested in teaching typical undergraduate courses, such as physical, inorganic, and organic chemistry. Additionally, I would like to establish upper-level courses and laboratories that require students to draw on their previous coursework to develop the concepts and tools needed to contribute to the field of organic materials chemistry.

Abstract Title: *Hydrogen and methane storage in a phthalocyanine 2D covalent...*

INOR Division

**63. Shivaiah Vaddypally;** Department of Chemistry, Temple University, 130 Beury Hall, 1901 N. Broad St., 12th St., Philadelphia, PA, 19122; [shivaiah@temple.edu](mailto:shivaiah@temple.edu), [shiva.vaddypally@gmail.com](mailto:shiva.vaddypally@gmail.com); Osmania University, Hyderabad, India (BS., 1996; B.S., 1999); University of Hyderabad, India (M.S., 2001; Ph.D., 2006), Prof. Samar. K. Das, Interactions of metal ions, metal complexes, and organic ligands with polyoxometalates: Synthesis, structure, and spectroscopic studies; Postdoctoral Researcher at Boston College (2007–2009), Prof. William Armstrong, Modeling bioinorganic clusters relevant to Photosystem II; Joint Postdoctoral Researcher at Temple University (2009–present), Dr. Zdilla, Synthesis and reactivity of biological inspired metal clusters and nanochemistry; <http://astro.temple.edu/~mzdilla/research.html>.

I am seeking a teaching and research position at an undergraduate/graduate research institute. My research projects involve synthesizing bioinorganic models mimicking enzyme systems and functional MOF materials based on biocompatible bis-peptides and predesigned organic ligands. I have been training undergraduates and graduates whose work resulted in research publications in prestigious journals. Collaborative research proposals will help gain knowledge in multidisciplinary areas and help students in their personal career development. I have a certified teaching degree, whose course work taught me teaching skills. I will benefit the department with skills such as operating an X-ray machine and solving crystal structures.

Abstract Title: *Metal clusters toward bioinorganic models and functional materials*

INOR, PMSE Divisions

**64. Ursula J. Williams;** Department of Chemistry, University of Pennsylvania, 231 South 34th St., Philadelphia, PA 19104; ursulaw@sas.upenn.edu; Union College (B.S., 2009); University of Pennsylvania (Ph.D., anticipated May 2014); Dr. Eric J. Schelter, Rational synthesis and characterization of tetravalent cerium coordination compounds.

I am interested in engaging undergraduates in research that investigates the synthesis of metal coordination compounds and uses spectroscopy, small molecule crystallography, magnetometry, electrochemistry, and chemical reactivity to explore the effects of ligand environments on electronic structure and bonding. I have teaching experience in general chemistry and undergraduate inorganic chemistry courses, and I have mentored several undergraduates in the research laboratory. I am pursuing a teaching- and research-focused career at a primarily undergraduate institution, and I am passionate about implementing active learning to more effectively engage undergraduates in and out of the classroom.

Abstract Title: *Rational synthetic routes to a family of tetravalent cerium amido...*

INOR Division

**65. Arindam Chatterjee;**

Abstract Title: *Identification of novel, selective CDK5/p25 inhibitor: Structure...*

**66. O. Andreea Cojocaru;** Center for Green Manufacturing and Department of Chemistry/Box 870336, 3016 Shelby Hall, 250 Hackberry Lane, The University of Alabama, Tuscaloosa, AL 35487; oacojocaru@as.ua.edu; Al. I. Cuza University, Iassy, Romania (B.S., 2003; M.S., 2005); The University of Alabama, Tuscaloosa (Ph.D., 2011), Prof. A. J. Arduengo, III, Synthesis and chemistry of 4,5-functionalized imidazoles; Postdoctoral Fellow at Center for Green Manufacturing and Department of Chemistry, The University of Alabama (June 2011–present), Prof. Robin D. Rogers, Herbicidal ionic liquids, active pharmaceutical ingredients in ionic liquid form, energetic ionic liquids.

My goal is to obtain a tenure-track position at a PUI. Based on previous teaching experience, I believe in the education of students through several teaching styles, such as encouraging active learning with discussions and group exercises as well as preparing short presentations on course-related topics, providing practice materials with a wide range of difficulty, and using visual demonstrations during class. I intend to develop a research program based on using ionic liquid technology, with a focus on developing new applications for biorenewable materials within waste remediation, and I hope to overcome the disadvantages of currently used solid-state pharmaceuticals.

Abstract Title: *Ionic liquid forms of active pharmaceutical ingredients in drug delivery*

MEDI, ORGN, ENVR Divisions

**67. Jie Zhou;** Department of Chemistry and Biochemistry, University of Maryland, College Park, 091 Chemistry Building, College Park, MD 20742; (+1) 301-405-7453, jzhou@umd.edu; Nanyang Technological University, Singapore (B.S., 2009); University of Maryland, College Park (Ph. D., anticipated 2014), Dr. Herman O. Sintim, c-di-GMP signaling in bacteria—New opportunities for the development of anti-biofilm drugs; <http://sites.google.com/sites/jzhouumd>.

I am seeking a faculty position at a primarily undergraduate institution that values teaching and research in equal measure and emphasizes global education. I have two-year teaching experience in undergraduate laboratory courses and mentoring undergraduate students for their research. My current research focuses on cyclic dinucleotides-related bacterial signaling, and especially on the innovation and development of anti-biofilm drugs. As a future chemical biologist, I plan to bring undergraduate students into the chemistry–biology interdisciplinary field, using not only my teaching and research experience, but also the cultural diversity and bilingual advantages I bring with me.

Abstract Title: *C-di-GMP signalling in bacteria: New opportunities for the...*

MEDI, BIOL Divisions

**68. Stephen Chamberland;** Department of Chemistry, Central Washington University, 400 E. University Way, Ellensburg, WA 98926; 509-963-1126, [chambers@cwu.edu](mailto:chambers@cwu.edu); Boston College (B.S., *cum laude*, 1999); University of California, Irvine (Ph.D., 2005), Prof. Keith Woerpel, Stabilization of particular conformers of six- and eight-membered ring oxocarbenium ions by remote stereocontrol leads to the stereoselective synthesis of small- and medium-ring ethers; Postdoctoral Fellow at Colorado State University (2005–2008), Prof. Robert M. Williams, Chemical synthesis of putative early- and late-stage biosynthetic intermediates of FR-900482 and mitomycin C; Assistant Professor of Chemistry at Central Washington University (2008–present), Principal Investigator, Total synthesis of biologically active natural products.

I am selectively seeking a faculty position at a research-intensive, primarily undergraduate or Ph.D.-granting institution (private or public) that expects teaching excellence. Mentoring 19 research assistants, including 2 honors students and 1 M.S. student, has led to publications and presentations at local and national venues. Grant-writing supports my research into the total synthesis of novel anticoagulants and anticancer compounds. Strong evaluations highlight five years of experience teaching undergraduate and graduate organic chemistry lecture and lab courses. My primary pedagogical goal is to instill a love of learning in each student while emphasizing critical thinking, conceptual understanding, accountability, and hard work.

Abstract Title: *Application of a straightforward approach to incorporate terminal...*

ORGN, MEDI Divisions

**69. Sandipan Dawn;** Conte National Center for Polymer Research, Department of Polymer Science and Engineering, University of Massachusetts, Amherst, 120 Governors Dr., Amherst, MA 01003; [sdawn@polysci.umass.edu](mailto:sdawn@polysci.umass.edu); University of Calcutta, India (B.S., M.S., 2003); University of South Carolina (Ph.D., 2012), Prof. L. S. Shimizu, Functional nanomaterials from bis-urea macrocycles; Postdoctoral Researcher at Conte National Center for Polymer Research, Department of Polymer Science and Engineering, University of Massachusetts, Amherst (2012–present), Prof. H. Bermudez, Patterning on block copolymer thin films, and Nanotechnology-based screening for carcinogen adducts.

I am interested in establishing a research program in organic chemistry–nanomaterial interphase with biological applications. As per my integrated background in chemistry, nanotechnology, and biomaterials, I want to train students in collaborative research using different branches of chemical sciences and in academia–industry overlaps. My research thrust will be: a) Film-based patterned biomaterials with antibody fragments for sensor applications, b) Self-assembled polymeric drug delivery vehicles, and c) Designing and synthesizing new functional materials for energy storage. As an experienced teacher, I want to develop a graduate-level course in “Functional Materials” along with basic chemistry and biochemistry courses.

Abstract Title: *Self-assembled functional nanomaterials from bis-urea macrocycles...*

ORGN, PMSE, BIOL, POLY Divisions

**70. Thomas J. Fisher;** Department of Chemistry and Biochemistry, 1118 NW 100 W. 18th Avenue, Columbus, OH 43210; 419-343-6569, thomas.j.fisher.chem@gmail.com; Bowling Green State University (B.S., 2007); University of Nebraska–Lincoln (Ph.D., 2012), Prof. Patrick H. Dussault, Part I: New reactions of alpha-oxygenated hydroperoxides, Part II: Design, synthesis, and applications of novel twin-chain amphiphiles; Postdoctoral Research Associate at The Ohio State University (2013–present), Prof. Anita E. Mattson, Development of new hydrogen bond donor organocatalytic methods targeted toward the total synthesis of biologically active and interesting scaffolds; <http://www.linkedin.com/pub/thomas-j-fisher/36/889/b13/>.

I am interested in working for a research-focused organization, whether at an R-1 type university or a smaller master's or bachelor's degree granting institution. Establishing a stimulating and significant research effort is paramount to my interests; this goal also facilitates any inherent teaching requirement. My research program would center on developing new synthetic methods in organic chemistry to create materials of interest ranging from biologically relevant frameworks to molecular organic materials. Imparting unique approaches to problem solving (e.g., using principals of organic chemistry for problems typically encountered by engineers/material scientists) will produce diverse students trained for interdisciplinary scientific research.

Abstract Title: *Hydrogen bond donor organic catalysts for the discovery of new...*

ORGN Division

**71. Nusrah Hussain;** Department of Chemistry, University of Pennsylvania, 231S 34th St., Philadelphia, PA 19104; [nusrah@sas.upenn.edu](mailto:nusrah@sas.upenn.edu); Bard College, Annandale-on-Hudson, NY (B.A., 2009); University of Pennsylvania (Ph.D., anticipated June 2014), Dr. Patrick J. Walsh, I. Palladium-catalyzed C(sp<sub>3</sub>)-H arylation via deprotonative cross-coupling processes, II. Chemoselective and diastereoselective C–C, C–O and C–N bond-forming reactions.

My research interests lie in developing new methodologies at the intersection of organic and organometallic chemistry. I am currently interested in metal-catalyzed cross-coupling reactions to form C–C bonds. I have held several laboratory TA positions for general and organic chemistry at Bard College and the University of Pennsylvania. I have a deep passion for teaching. I seek to teach and mentor students in academia.

Abstract Title: *Palladium-catalyzed deprotonative cross-coupling process of...*

ORGN Division

**72. Laura C. Miller;** 106 Frick Laboratory, Princeton University, Princeton, NJ 08544; [lcmiller@princeton.edu](mailto:lcmiller@princeton.edu); Macalester College (B.A., 2005); University of California, Berkeley (Ph.D., 2010), Prof. Richmond Sarpong, Studies toward total synthesis of the cyathane and cyanthiwigin diterpenes; Postdoctoral Research Associate at Princeton University (2010–present), Prof. Martin Semmelhack and Prof. Bonnie Bassler, Modulation and investigation of quorum sensing enabled by the design and synthesis of small molecules.

Leveraging techniques from organic chemistry and biochemistry, I will interrogate biological systems and disease at a primarily undergraduate or master's degree granting institution. I plan to develop a vibrant research program where students will investigate antivirulence strategies against bacteria using organic chemistry, biochemistry, and molecular biology. I've assisted teaching organic chemistry, biochemistry, and chemistry pedagogy courses at Berkeley and Princeton, where I also mentored a number of undergraduate researchers. I am passionate about engaging students in the classroom and the lab. I'm also committed to nurturing a love of science in both the students and the community through outreach activities.

Abstract Title: *Blocking virulence: Disruption of quorum sensing in Pseudomonas...*

ORGN, MEDI, BIOL Divisions

**73. Maxim Ratnikov;** Department of Chemistry, The Scripps Research Institute, 10550 North Torrey Pines Road, La Jolla, CA 92037; [ratnikov@scripps.edu](mailto:ratnikov@scripps.edu); Higher Chemical College, Moscow (B.S./M.S., Chem, 2007); University of Maryland (Ph.D., Chem, 2012), Dr. Michael Doyle, Dirhodium caprolactamate catalyzed oxidations by *tert*-butyl hydroperoxide: From mechanism to new methodologies; Postdoctoral Researcher at The Scripps Research Institute (2012–present), Dr. Valery Fokin, Investigation of on water catalysis toward sustainable manufacturing.

I seek a tenure-track position focusing on excellence in teaching and student research. During a two-year Graduate Assistance in Areas of National Need (GAANN) Fellowship, I initiated adoption of online homework for organic chemistry lectures, developed curriculum for a new laboratory course, and was exposed to teaching a 200-student class. I strive to involve students in research and have supervised five undergraduates—teaching transferable skills through research and preparing them for life after graduation. I am interested in research employing organic chemistry to design materials for eliminating heavy metals from water and to introduce new properties to polyethylene and polystyrene.

Abstract Title: *Water as a heterogeneous liquid catalyst: From mechanism to...*

ORGN Division

**74. Kinkini Roy;** Silvio O. Conte National Center for Polymer Research, Department of Polymer Science and Engineering, University of Massachusetts, Amherst, Massachusetts, 01002; [kinkiniroy@polysci.umass.edu](mailto:kinkiniroy@polysci.umass.edu); University of Calcutta, India (B.S., M.S. 2003); University of South Carolina–Columbia (Ph.D., 2012), Prof. L. S. Shimizu, Synthesis and recognition properties of functionalized nanomaterials from pyridyl urea macrocycle; Postdoctoral Researcher at the Silvio O. Conte National Center for Polymer Research, Department of Polymer Science and Engineering, University of Massachusetts, Amherst (2012–present), Prof E. Bryan Coughlin, Phosphazene oligomers and polymers as low-viscosity electrolytes for lithium ion batteries, and Base cleavable block copolymers for use in photolithography.

My research program will emphasize synthesizing new material—including polymer, nanomaterial, and composite—that will have numerous applications in therapeutics as a drug delivery vehicle. I will develop a macromolecular system by supramolecular self-assembly that will have potential application from sensor to ion exchange membrane. I will develop fire-safe, flexible material that will reduce the number of deaths in aircraft accidents and military transportation. From my vast experience in organic, material science, polymer, and bioorganic chemistry, I will develop a multidisciplinary lab and train my graduate students, undergraduates, and postdoctoral scholars for academia as well as industry research.

Abstract Title: *Functionalized nanomaterials from pyridyl urea macrocycles and...*

ORGN, PMSE, POLY, BIOL Divisions

**75. Biswajit Saha;** Department of Chemistry, North Central College, 30 N. Brainard St., Naperville, IL 60540; bsaha75@gmail.com; Indian Institute of Technology Kanpur (M.S., 1997); Kyushu University, Japan (Ph.D., 2003); Prof. Tsutomu Katsuki, Metallocalen catalyzed asymmetric intramolecular cyclopropanation; Postdoctoral Researcher at The Ohio State University (2003–2007), Prof. T. V. RajanBabu, Development of industrially useful catalytic reactions; Visiting Assistant Professor at North Central College [Year not provided].

I seek a tenure-track position at a primarily four-year liberal arts institution. I'm creative, energetic, enthusiastic, and dependable, with extensive experience in teaching freshman to senior chemistry courses. An experienced, multicultural teacher and researcher, I can promote academic and professional excellence among my students and prepare them for future leadership in a global context. I have successfully mentored and supervised students to succeed in the classroom and in laboratory research. My research goal is to develop environmentally sustainable green catalytic organic reactions. I'll add value to any liberal arts college by assessing challenges in student learning and improving teaching solutions.

Abstract Title: *Silver(I)-catalyzed regioselective cyclization reactions*

ORGN, MEDI, ENVR Divisions

**76. Andrew G. Schafer;** Department of Chemistry and Biochemistry, The Ohio State University, 88 W. 18th Ave., EL 4087, Columbus, OH 43210; aschafer@chemistry.ohio-state.edu; John Carroll University (B.S., 2009); The Ohio State University (Ph.D., anticipated 2014), Dr. Anita E. Mattson, Design and development of silanediols as a new class of hydrogen bond donor catalysts; [www.linkedin.com/pub/andrew-schafer/67/63/607/](http://www.linkedin.com/pub/andrew-schafer/67/63/607/).

Teaching is my passion, and I am seeking a position at an undergraduate institution where teaching is at the forefront. My teaching experience includes undergraduate organic lecture and lab, general chemistry lab, and a graduate synthetic organic course. I am inspired by the opportunity to lead organic lectures and labs and to develop advanced undergraduate and nonmajors chemistry courses. My research interests include organocatalytic synthesis and methodology appropriate for undergraduate researchers. My goal is to build a program to provide undergraduates a practical foundation for their postgraduate careers by incorporating original research into the development of creative, critical-thinking individuals.

Abstract Title: *Silanediols as catalysts for nitroalkene activation*

ORGN Division

**77. Buck L. H. Taylor;** Department of Chemistry and Biochemistry, University of California, Los Angeles, 607 Charles E. Young Drive E., Los Angeles, CA 90095; [bucktaylor@ucla.edu](mailto:bucktaylor@ucla.edu); Willamette University (B.A., 2007), Prof. Sarah R. Kirk; University of California, Irvine (Ph.D., Pedagogical Fellow, 2012), Prof. Elizabeth R. Jarvo, Development of stereospecific nickel-catalyzed cross-coupling reactions; NIH Postdoctoral Fellow at UCLA (2012–present), Prof. Kendall N. Houk, Computational investigation of metal-catalyzed allylation and olefin-metathesis reactions; <http://bucktaylor.bol.ucla.edu/>.

I plan to teach and direct research at a primarily undergraduate institution. I will establish a research program to answer mechanistic questions in organic reaction development and catalysis using computational and experimental techniques. My research will complement the organic chemistry curriculum and help undergraduate researchers understand complex reaction mechanisms and catalyst design. My experience as a lecturer at UCLA (sophomore organic chemistry), instructor at UCI (Research Methods for Science Teachers), TA-training fellow, and mentor for undergraduate research in both synthetic organic and computational chemistry have been outstanding preparation for a faculty position at a research-active PUI.

Abstract Title: *Development of stereospecific nickel-catalyzed cross-coupling reactions...*

ORGN, INOR, COMP Divisions

**78. Kristopher V. Waynant;** 405 N. Mathews Dr., Beckman Institute, UIUC, Urbana, IL 61801; [kwaynant@illinois.edu](mailto:kwaynant@illinois.edu); Virginia Tech (B.S., Biochem; B.A., Chem, 2002); New Mexico State University (M.S., Ph.D., Org Chem, 2008), Dr. James W. Herndon, Fischer metallocarbene methodology; Postdoctoral Researcher at Oregon State University (2009–2010), Dr. James D. White, Complex molecule total synthesis; Postdoctoral Teaching and Research Fellow at Colgate University (2010–2012), Dr. Ernie G. Nolen, Synthesis of carbon-linked glycomimetics; Postdoctoral Researcher at the University of Illinois at Urbana-Champaign (2012–2013), Dr. Paul V. Braun, Synthesis of polymer brush gradients and remediation of organophosphates.

I've had the opportunity to experience a variety of academic settings and believe that I have adapted myself to each and proved successful. This diversity allows me to be able to tailor my research and teaching goals to highlight specific departments' strengths. I do enjoy teaching, having taught at Colgate, but I would also like to continue to educate students through research work to prepare them for their next challenges. As a synthetic chemist, I can see many projects in organic methodology, complex molecule synthesis, and monomer modification for new materials applications.

Abstract Title: *Carbenes, cancer, and chemical transport*

ORGN, POLY, PMSE Divisions

**79. Jing Yi;** Department of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN 47907; jing.yi02@gmail.com; Ocean University of China (B.S., 2006); Wuhan University (M.S., 2008), Dr. Zixing Shan, (I) Preparation of arylboronic acid, (II) Enrichment of the excess enantiomer in nonracemic 1,1'-Bi-2-naphthol through achiral selective complexation; North Dakota State University (M.S., 2010), Dr. Wenfang Sun, Synthesis and photophysics of platinum(II) terdentate and bidentate complexes; Research Assistant at Purdue University Department of Chemistry (2010–present), Dr. Mahdi Abu-Omar, Different applications of rhenium catalysts.

I seek a position in organic catalysis allowing me to teach and perform independent research as a faculty member at a research-oriented comprehensive university. I'm interested in developing organometallic catalytic systems (boron-, platinum-, rhenium-catalyzed organic reactions). A motivated organic chemist with seven years' hands-on research experience in academia and industry, I've worked on organocatalysis, photochemistry, nonlinear optical materials, and total synthesis of medicinal intermediates. My work has been published in *ChemSusChem*. I enjoy teaching and have experience as a TA for general and organic chemistry courses. I'm pleased to have been nominated for an outstanding TA award in fall 2011.

Abstract Title: *Applications of rhenium catalysts*

ORGN, INOR, CATL, ENVR Divisions

**80. Ming-Wei Chen;** Department of Chemistry, University of Illinois at Urbana-Champaign, 505 South Mathews Ave., Urbana, IL 61801; mingchen@illinois.edu; National Chiao Tung University, Hsinchu, Taiwan (B.S., 2000); National Tsing Hua University, Hsinchu, Taiwan (M.S., 2002), Dr. I-Chan Chen (Chem), Spectroscopy, quantum beats and dynamical study at near formation threshold for fragment HCO of glyoxal and acetaldehyde; The Ohio State University, Columbus (Ph.D., 2011), Dr. Terry A. Miller (Chem Physics), Laser spectroscopy studying organic and inorganic intermediates in the atmospheric oxidation process; Postdoctoral Research Associate, University of Illinois at Urbana-Champaign (2011–present), Dr. Dana D. Dlott, Exploring energy concentration in energetic materials initiated by weak energies via MWIR/thermal imaging microscopy; <https://sites.google.com/site/mingweichen1195/>.

Based on interdisciplinary education in chemistry and physics, I have been interested in discovering the structure and mechanism of chemical reaction at the molecular level. I led students and developed laser spectroscopy techniques to study reactive intermediates produced by nature or human activities, and published in leading journals. Recently, I've developed new imaging technology to study energy concentration in energetic materials. I also taught general and physical chemistry recitations and labs. Gathering all research and teaching experiences, I look forward to getting a faculty position in a university or college to continue on research and encourage students studying physical science.

Abstract Title: *Laser spectroscopy and imaging techniques studying chemicals and...*

PHYS, ANYL, ENVR Divisions

**81. Borislav L. Ivanov;** Department of Physics and Astronomy, 6301 Stevenson Science Center, Vanderbilt University, Nashville, TN 37235-1807; [borislav.ivanov@vanderbilt.edu](mailto:borislav.ivanov@vanderbilt.edu); [Undergraduate information not provided]; University of Chemical Technology and Metallurgy, Sofia, Bulgaria (Ph.D., 1994), [Adviser's name not provided], Laser chemical vapor deposition of thin Al layers from organometallic precursors by copper vapor laser; Research Assistant Professor at Vanderbilt University (2003), [Adviser's name and topic not provided]; Research Associate Professor at Vanderbilt University (2009–present), [Adviser's name not provided], Laser-induced materials chemistry and laser–materials interactions using pulse lasers with pulse duration from microseconds to femtoseconds and wavelength from mid-IR to blue range of the visible spectra.

I'm also strongly interested in energy-related materials chemistry in forming anodes and cathodes for Li ion batteries and in catalysis for fuel cells and laser micromachining for micro fuel cells, as well as synthesizing new superconductor compounds in the upper-left corner of the periodic table. Applying laser technologies in microelectronics and medicine (laser surgery and drug delivery) also interests me. I seek a tenure-track position strongly accentuating excellence in research and education in a research-oriented university. I can teach courses in inorganic, physical, and materials chemistry; also technology of semiconductor materials and integrated circuits, materials science and laser–materials interactions.

Abstract Title: *Materials chemistry by pulse visible and IR lasers: CPCD...*

PHYS, COLL, INOR, PMSE Divisions

**82. Yongjun Li;** Department of Chemistry, Columbia University, 3000 Broadway, New York, NY, 10027; [yl2560@columbia.edu](mailto:yl2560@columbia.edu); Nanjing University of Science and Technology (B.E., 1998); University of Florida (Ph.D., 2009), Dr. Kirk Schanze, Photophysics of conjugated organometallic systems: Photoinduced electron transfer and energy transfer, triplet exciton delocalization, and phosphorescent organogelators; Postdoctoral Associate at Columbia University (2009–present), Dr. Nicholas Turro, Synthesis and spin chemistry of nitroxide-labeled guest@host systems; electron magnetic resonance study of spin labeled brush polymers; analysis and photophysical characterization of photoresponsive polymers.

My future research will focus on design, synthesis, and photophysical characterization of organic materials and polymers with potential applications in the energy or biomedical field. I have taught undergraduate student courses and labs and supervised both undergraduate and graduate students in their research studies. I am interested in a faculty position in a research-oriented university.

Abstract Title: *EPR study of nitroxide-labeled brush polymers*

PHYS, ORGN, ANYL Divisions

**83. Gerrick Lindberg;** Department of Chemistry, University of Chicago, Chicago, IL 60637; gerrick@uchicago.edu; Oregon State University (B.S., Adv Chem, minors Math and History, 2005); Boston University (M.A., 2009; Ph.D., 2011), Prof. Feng Wang, Molecular dynamics investigation of the free energy of melting of methane clathrate and ice Ih; Postdoctoral Scholar at the University of Chicago (2010–present), Prof. Gregory A. Voth, Multiscale modeling of hydroxide solvation and transport in anion exchange membranes and other basic environments.

I am seeking a position at a primarily undergraduate institution with opportunities to develop as a teacher and researcher. I value teaching because chemistry is central to understanding our world, and it can help students develop the ability to think critically and creatively. My research interests focus on applying theoretical and computational chemistry to advance renewable energy technologies, specifically developing novel energy storage materials and energy conversion methods. In addition to its wide-reaching implications for society, this research will expose students to many modern methods in statistical mechanics, thermodynamics, and supercomputing.

Abstract Title: *Guiding the development of anion exchange membrane fuel cells...*

PHYS, COMP, FUEL Divisions

**84. Josh J. Newby;** Department of Chemistry and Biochemistry, Swarthmore College, 500 College Avenue, Swarthmore, PA 19081; (610)-690-6893, [jnewby1@swarthmore.edu](mailto:jnewby1@swarthmore.edu); Eastern Illinois University (B.S., 2004); Purdue University (Ph.D., 2009), [Adviser's name not provided], Spectroscopic characterization of aromatic species important to the atmosphere of Titan; Postdoctoral Associate at Purdue University (2009–2011), [Adviser's name not provided], Development of analytical materials and methods using self-assembled silica nanostructures; Visiting Assistant Professor of chemistry at Swarthmore College (present); [www.swarthmore.edu/academics/josh-newby.xml](http://www.swarthmore.edu/academics/josh-newby.xml).

I am seeking a tenure-track position in physical chemistry. I would prefer an undergraduate institution, but I'm open to master's degree programs. At Swarthmore College, I have taught courses in general chemistry, quantum mechanics, thermodynamics, and associated labs. I've had a great experience in an undergraduate environment and I want more! While at Swarthmore, I received technology grants to incorporate Web-based tools for learning and assessment. I currently advise an undergraduate research group that uses high-resolution spectroscopy to characterize natural product molecules. I want to build a spectroscopic research program that can build on my past and present research experience.

Abstract Title: *Spectroscopic analysis of a natural product: Anethole*

PHYS, ANYL Divisions

**85. Christina M. Ragain;** Department of Chemistry and Biochemistry, The University of Texas at Austin, 105 E. 24th St. Stop A5300, Austin, TX 78712-1224; [cmragain@utexas.edu](mailto:cmragain@utexas.edu); The University of North Carolina at Greensboro (B.S., 2004); Yale University (M.S., 2006); The University of Texas at Austin (Ph.D., anticipated 2014), Lauren J. Webb (Chem), Measuring electrostatic fields at protein interfaces using vibrational Stark effect spectroscopy.

Chemistry is an apprenticeship art; this is an idea I tried to instill in my students while serving as a lecturer in chemistry at The University of Texas at Tyler. I created an outreach program targeted at bringing chemistry to the community and redesigned several courses, including the introductory chemistry series and biochemistry lab. My desire to have a greater impact led me to pursue my Ph.D., and I now seek a full-time faculty position at a teaching-focused institution. I will incorporate research into the everyday classroom experience as well as create a research program designed with undergraduates in mind.

Abstract Title: *Measuring electrostatic fields at protein interfaces using vibrational...*

PHYS, BIOL, CHED Divisions

**86. Annette Raigoza;** Department of Chemistry, The University of Texas at Austin, 105 E. 24th St. STOP A5300, Austin, TX 78712; [araigoza@austin.utexas.edu](mailto:araigoza@austin.utexas.edu); University of Texas of the Permian Basin (B.S., 2002); University of Notre Dame (M.S., 2006); Dr. Dennis C. Jacobs (Chem), Metal-insulator-metal devices; University of Notre Dame (Ph.D., 2012); Dr. S. Alex Kandel (Chem), Scanning tunneling microscopy studies of mixed self-assembled monolayers; Postdoctoral Fellow at The University of Texas at Austin (2012–present), Dr. Lauren J. Webb (Chem), Chemical preparations of biomimetic surfaces to control protein–surface interactions.

Self-assembled monolayers (SAMs) are simple systems that show great potential for a wide range of technologies. Using scanning probe microscopy techniques and spectroscopic methods, I plan to expand the collection of currently attainable SAM surfaces. I am also interested in the interactions of biological materials and structured surfaces. I have taught chemistry classes as an adjunct instructor at St. Philip's College. Additionally, I have enjoyed mentoring numerous high school, undergraduate, and graduate students on independent research projects. I would like to earn a faculty position in a primarily undergraduate institution, teaching and directing undergraduate research.

Abstract Title: *Self-assembled monolayers: A simple foundation for fundamental and...*

PHYS, COLL Divisions

**87. David W. H. Swenson;** van 't Hoff Institute for Molecular Sciences, Universiteit van Amsterdam, Postbus 94157, 1090GD Amsterdam, The Netherlands; [dwhs@hyperblazer.net](mailto:dwhs@hyperblazer.net); Colorado College (B.A., Chem, French Lit, Phys, 2003); Université Louis Pasteur, Strasbourg (D.E.U.G., Math, 2005); University of California, Berkeley (Ph.D., Chem, 2011), Prof. William H. Miller, New methods for semiclassical dynamics; Postdoctoral Fellow at Tel Aviv University (2011), Prof. Eran Rabani, Semiclassical treatment of molecular electronics; Postdoctoral Fellow at Universiteit van Amsterdam (2012–present), Prof. Peter G. Bolhuis, Methods for studying rare events, especially correlated rare events; <http://www.hyperblazer.net/>.

I want my work to push the frontiers of what can be accurately simulated with molecular dynamics. Recently, I've developed three techniques to do that: tools to reproduce the dynamics of discrete quantum systems using continuous classical models, tools to describe correlated rare events, and tools to study dynamical quantum coherences. I'd like to build a research group in which undergraduate and graduate students work together both to develop novel methods to simulate complex systems at longer timescales and with quantum effects, and to apply those methods to significant problems such as energy transfer and molecular recognition in biological systems.

Abstract Title: *Beyond basic molecular dynamics: New tools for the study of molecules...*

PHYS, COMP Divisions

**88. Bryan M. Wong;** Nanoelectronics and Nanophotonics Group, Sandia National Laboratories, Livermore, CA 94551; usagi@alum.mit.edu; Rice University (B.S., 2001); M.I.T. (Ph.D., 2007), Prof. Robert W. Field, Quantum chemistry for spectroscopy; Senior Member of the Technical Staff at Sandia National Laboratories (2007–present), First-principles calculations of energetic nanomaterials; <http://alum.mit.edu/www/usagi>.

I am a senior member of the technical staff in the Nanoelectronics and Nanophotonics group at Sandia National Laboratories. I received my B.S. degrees in physics and chemistry (summa cum laude, 2001) from Rice University and received a Ph.D. in chemical physics from the Massachusetts Institute of Technology (M.I.T., 2007). I specialize in first-principles calculations for predicting electronic properties of photovoltaic materials, functionalized carbon nanotubes, graphene-based materials, and semiconductor nanowires. I have published more than 60 scientific journal articles within the areas of materials science, physics, and chemistry, and I am interested in a faculty position at a research-intensive university.

Abstract Title: *Energy transfer in molecular photovoltaics, carbon nanotubes...*

PHYS, COMP Divisions

**89. Lai Xu;** Department of Chemistry, Missouri University of Science and Technology, 1870 Miner Circle, Rolla, MO 65409; xula.mst@gmail.com; Peking University, Beijing (B.S., 2005); University of California, Los Angeles (Ph.D., ACS Chemical Computing Group (CCG) Research Excellence Award, 2011), Prof. Kendall N. Houk, Dynamics and mechanisms of organic reactions; Postdoctoral Research Associate at Texas Tech University (2011–2012), Prof. William L. Hase, Analytical potential energy surface of organic molecular reacting with TiO<sub>2</sub> surface; Postdoctoral Research Associate at Missouri University of Science and Technology (2012–present), Prof. Nicholas Leventis, Multiscale simulations of polymeric nanomaterials.

I seek a tenure-track faculty position at a research university. My primary research is directed toward using a theoretical and computational approach, in close collaboration with experimentalists, to investigate mechanisms ranging from small-molecule chemical reactions to large-scale materials. My long-term research plans seek to understand organic reactions, polymeric materials, and biological systems by multiscale simulations. My specific research plans involve the structure–properties study and dynamics of polymeric nanomaterials, with applications to gas storage and separation. For teaching, I wish to provide an environment for students to cultivate the capacity for scientific critical thinking.

Abstract Title: *Dynamics and timing: A tale of two studies*

PMSE, PHYS, ORGN, COMP Divisions

**90. Marjorie A. Kiechel;** Department of Materials Science and Engineering, Drexel University, Philadelphia, PA; +1-215-301-5518, [msa39@drexel.edu](mailto:msa39@drexel.edu); University of the Philippines (B.S., Food Sci, 2005); Ateneo de Davao University (M.S., Chem, CAR, 2008); Drexel University (M.S., Food Sci, 2011); Drexel University (Ph.D., Materials Sci & Eng, 2013), Dr. Caroline L. Schauer (M.S.E.) and Dr. A. Philipp Handel (Food Sci), Postprocessing of electrospun cationic polyelectrolyte fibers for filtration, food, and biomedical applications.

I am interested in working in a research-intensive university while developing novel materials from natural polyelectrolytes. Particularly, I plan on investigating their material nanodesign and characterization (FESEM, TEM, FTIR, NMR, XRD, UV-Vis, cellular assays, filtration profile, porosity tests) for food, wastewater treatment, and biomedical applications. I plan to continue teaching students, specifically women and minorities, and inspiring them to be responsible and passionate innovators. My long-term plan also involves taking on administrative duties and leading a dynamic team that will look into how the quality of science-engineering education would be able to meet the demands of industry, government, and academe.

Abstract Title: *Post-processing electrospun chitosan fibers for filtration applications*

PMSE, CARB, POLY, CELL Divisions

**91. Dimitrios Priftis;** Institute for Molecular Engineering, University of Chicago, 5735 S. Ellis Ave., Chicago, IL 60637; [dpriftis@uchicago.edu](mailto:dpriftis@uchicago.edu); Aristotle University of Thessaloniki, Greece (B.S., Chem, 2004); University of Athens, Greece (M.S., Poly Chem, 2006), Prof. N. Hadjichristidis, Synthesis and characterization of poly( $\epsilon$ -caprolactone) miktoarm star copolymers with the use of a multifunctional initiator; University of Athens, Greece (Ph.D., Poly Chem, 2009), Prof. N. Hadjichristidis, Polymer grafting of carbon nanotubes; Postdoctoral Research Associate at Department of Bioengineering, University of California, Berkeley (May 2010–November 2011), Prof. M. Tirrell, Polyelectrolyte complexes: Complex coacervation of polypeptides; Postdoctoral Research Associate at University of Chicago, (November 2011–April 2013) and Research Professional II (May 2013–present), Prof. M. Tirrell, Polyelectrolyte self-assembly materials driven by complex coacervation.

My research is driven by a strong curiosity to create and study new materials and target specific applications by bridging knowledge from various disciplines (i.e., chemistry, materials, physics, bioengineering). I am especially attracted by the design and development of soft materials through polymer synthesis and the use of supramolecular chemistry or self-assembly. My goal is to establish a strong, externally funded research program at a Ph.D.-granting institution. I have served as a teaching assistant for different undergraduate and graduate courses and mentored students in multiple research projects. I look forward to further opportunities to teach, inspire, and mentor.

Abstract Title: *Polymer-based soft materials: Coacervate assemblies, carbon nanotube...*

PMSE, POLY Divisions

**92. Fang Ren;** Department of Chemical and Environmental Engineering, Yale University, 9 Hillhouse Ave., ML 310, New Haven, CT 06510; [ren.fang.ren@gmail.com](mailto:ren.fang.ren@gmail.com); Huazhong University of Science and Technology (B.S., 2008); Yale University (M.S., 2009; Ph.D., 2013), Prof. Lisa D. Pfefferle (Che.E.) and Prof. Gary L. Haller (Che.E.), Property control of single-walled carbon nanotubes through synthesis; <http://www.fang-ren.com/>.

My major research interest is synthesizing 0D, 1D, and 2D nanomaterials for electronic and energy applications, such as solar cell, field effect transistors, topological insulators, spintronics, etc.—which involves catalyst design, nanomaterial fabrication, functionalization, and doping—and studying the fundamentals (local bonding structure, chemical state, nanoparticle size and composition, etc.) in order to explain the mechanisms of synthesis reactions. My research interests also include investigating effective characterization techniques for both catalysts and nanomaterials to further guide the synthesis. I want to find a postdoctoral position in a university, an institute, or a national lab in the New England Area.

Abstract Title: *Property control of single-walled carbon nanotubes through synthesis*

ENFL, PMSE Divisions

**93. Bret D. Ulery;** Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637; [bulery@uchicago.edu](mailto:bulery@uchicago.edu); University of Iowa, Iowa City (B.S., Biochem, 2006; B.S.E., Chem Eng, 2006); Iowa State University, Ames (Ph.D., Chem Eng, 2010), Prof. Balaji Narasimhan, Molecular design of nanoparticle-based delivery vehicles for pneumonic plague; Postdoctoral Fellow at the Institute for Regenerative Engineering (2010–2012), Prof. Cato Laurencin, Biomaterials design for local anesthetic delivery and musculoskeletal regenerative engineering; Postdoctoral Scholar at the University of Chicago (2012–present), Prof. Matthew Tirrell, Self-assembled peptide amphiphile micelles for vaccination and immunotherapeutic applications.

My independent research will focus on exploiting the physicochemical properties of biomaterials to yield desirable immunoengineering and tissue engineering outcomes. Using polymer chemistry, chemical engineering, and materials science principles, I will generate platform technologies capable of carrying out multifaceted biomodulatory effects. As a faculty member, I look forward to the opportunity to mentor and train researchers at all academic levels from high school students and undergraduates to graduate students and postdoctoral fellows. Ideally, I would like to work at a Ph.D.-granting university that values a balance of teaching and research.

Abstract Title: *Biomodulatory materials*

PMSE, POLY, BIOL Divisions

**94. Joseph R. Lott;** Department of Chemistry, University of Minnesota, 207 Pleasant St. SE, Minneapolis, MN 55455; 716-946-4469, [jrlott@umn.edu](mailto:jrlott@umn.edu); Rochester Institute of Technology (B.S., 2004; M.S., 2006), Dr. Thomas Smith, Reversible addition-fragmentation chain-transfer (RAFT) polymerization in grafting polymer chains from TiO<sub>2</sub> nanoparticles; Case Western Reserve University (Ph.D., [Year not provided]), Dr. Christoph Weder, Design, synthesis, and incorporation of functional additives into multilayered polymer films; Postdoctoral Associate at the University of Minnesota (2011–present), Dr. Timothy P. Lodge and Dr. Frank S. Bates, Investigating phase behavior, physics of gelation, and structure–property relationships in aqueous cellulose ethers.

I am seeking a tenure-track faculty position with an emphasis on research at both the undergraduate and graduate levels. My research interests involve exploiting the chemical and morphological control afforded by macromolecules to enable, activate, direct, and spatially segregate technologically relevant optical processes (stimuli responsive smart sensors, low-power photon upconversion, solar-driven energy production). I am passionate about teaching all areas of chemistry, but have a strong enthusiasm for materials-related topics. I would enjoy teaching undergraduate classes covering general, analytical, and organic chemistry. However, I am particularly interested in teaching upper-level courses such as polymer synthesis and characterization.

Abstract Title: *Manipulating light with polymeric materials*

POLY, PMSE Divisions

**95. Brett P. Fors;** University of California, Materials Research Laboratory, Santa Barbara, CA 93106; [fors@mrl.ucsb.edu](mailto:fors@mrl.ucsb.edu); Montana State University, (B.S., 2002); Massachusetts Institute of Technology (Ph.D., 2011), Prof. Stephen L. Buchwald, Development and applications of Pd catalysts for C–N cross-coupling reactions; Elings Prize Postdoctoral Fellow at the University of California, Santa Barbara (2011–present), Prof. Craig J. Hawker, Spatial and temporal regulation of a controlled radical polymerization by light.

I am seeking a faculty position at a Ph.D.-granting institution where I can build an interdisciplinary and collaborative research program. My research will focus on using organic synthesis and catalysis as tools to address challenges in polymer and materials science. Equally important, a priority of my career will be educating and training future scientists. Through mentorship, teaching, and an edifying environment, I want to prepare graduate and undergraduate students to be independent and productive scientists, as well as provide them with the skills necessary to accomplish their own career goals.

Abstract Title: *Spatial and temporal regulation of a controlled radical polymerization...*

ORGN, POLY, PMSE Divisions

**96 Alireza Abbaspourrad**

Abstract Title: *Polymeric microcapsules with programmable active release*

**97. Libin Xu;** Department of Chemistry, Vanderbilt University, 7330 Stevenson Center, Station B 351822, Nashville, TN 37235; libin.xu@vanderbilt.edu; Nankai University, Tianjin, China (B.S., 2002); University of Illinois at Chicago (Ph.D., 2007), Dr. Martin Newcomb, Mechanism of free radical reaction; Research Associate (2007–2009), Senior Research Associate (2009–2010), Research Assistant Professor (2010–2012), Research Associate Professor (Jan 2013–present) at Vanderbilt University, Dr. Ned A. Porter, Lipid peroxidation and human diseases.

My research lies at the interface of the chemistry and biology of lipid peroxidation. I am particularly interested in elucidating the reaction mechanism of peroxidation of sterols and the underlying roles of the oxidation products in different human diseases. I am the PI of an NIH Pathway to Independence Award (K99) and a pilot grant from the NIEHS-funded Vanderbilt University Center in Molecular Toxicology. I am seeking a tenure-track position in a Ph.D.-granting institution. I will strive to build a continuously growing, externally funded, and independent research program that is well set up for student and postdoctoral training.

Abstract Title: *Free radical oxidation of 7-dehydrocholesterol and its role in human...*

ORGN, TOXI, BIOL, ANYL Divisions

## AEI 1

### High pressure sterilization of milk rich in conjugated linoleic acid

**Sergio Martínez-Monteagudo**, simartin@ualberta.ca. University of Alberta, Edmonton, Alberta T6G 2P5, Canada

Consumption of conjugated linoleic acid (CLA) has been positively correlated with health-promoting and disease-preventing properties. Unfortunately, CLA in milk suffers significant losses through oxidation during thermal treatments. The application of high pressure to a preheated sample reduces the severity of thermal treatments, preserving the biological activity of functional compounds. Indeed, our own results showed that milk rich in CLA can be treated with high pressure sterilization, resulting in minor losses of CLA. The objective of this study was to determine the oxidation kinetics of CLA in enriched milk during high pressure sterilization. In addition, the effect of high pressure sterilization treatment on the kinetic of some quality indicators was studied (lactulose formation, enzyme and spore inactivation). The kinetics were investigated in milk rich in CLA (36 mg/g) treated at a temperature range of 90-120°C, pressure range of 0.1-600 MPa and holding time range of 0-60 min. The kinetic analysis indicates that CLA is being isomerized under pressure in the presence of oxygen and the use of phenolic antioxidants not only enhances the retention for CLA but also avoid the isomerization by quenching the dissolved oxygen. We have found the processing conditions at which commercial sterilization was achieved (6-log of *B. amyloliquefaciens*) and 90% of the CLA was retained. The outcomes from this work are of great relevance for developing functional sterile beverages.

## AEI 2

### How do lipids oxidize in foods?

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Due to increased reformulation of foods with unsaturated oils, the food industry has encountered considerable challenges in stabilizing foods using approaches based on traditional lipid oxidation theory. Thus, it is becoming increasingly clear that the current understanding of lipid oxidation is incomplete and potentially inaccurate. This research investigates alternate pathways of lipid oxidation involving both peroxy (LOO<sup>•</sup>) and alkoxyl (LO<sup>•</sup>) radicals and looks for competing reactions such as internal rearrangements, scission, and addition that compete with classical hydrogen abstraction in a methyl linoleate model system. Gas chromatography (GC-FID) was used to track volatile product formation, comparing static headspace, SPME and thermal desorption (dynamic headspace) techniques. While current understanding accepts equal reactivity C9 and C13 of linoleic acid, volatile products arise predominantly from the CH<sub>3</sub> terminus, with a preference for scissions close to the double bond. Pentane is by far the major product, and products much more numerous than expected alkoxyl radical

scission products were detected. In these closed systems, some products did not accumulate continuously but rather cycled (increase then decrease) repeatedly, and this pattern was matched exactly by non-volatile products. However, other products did not cycle. Overall, these results emphasize that lipid oxidation is dynamic and products continue to react, and verify that reactions pathways other than hydrogen abstraction are active. Results also raise questions about use of headspace analyses to judge extent of lipid oxidation and derive complex reaction mechanisms. An integrated scheme showing how multiple pathways are simultaneously active and competing with each other is proposed.

### **AEI 3**

#### **Understanding the evolutionary relationship of protein tyrosine phosphatases and adaptor domains**

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Adaptor domains are now a common feature of signaling proteins and are broadly understood to redirect the activity of a catalytic domain to otherwise poor substrates. The specificity of an enzyme is influenced both by the structure of the active site of the enzyme and the presence of adaptor domains that localize the enzyme with respect to substrates. The interconnected properties of the catalytic and adaptor domains influence the overall specificity of the enzyme, and yet, it remains poorly understood how the catalytic activity has evolved with the introduction of the adaptor domains. Indeed, an understanding of this relationship could prove beneficial in understanding biological networks, the identification of targets for drug discovery, and the improvement of methods for functional annotation of gene products.

In this work, we focus on a class of highly conserved protein tyrosine phosphatase (PTP) domains that are found in proteins that include or omit SH2 adaptor domains. SH2 adaptor domains bind to peptide motifs containing a phosphorylated tyrosine residue and PTP. PTPs represent an effective model system for identifying a correlation between the addition of an adaptor protein to a gene and a loss of enzyme activity that accompanies this addition. We studied two PTPs with very different kinetic efficiency, PTP1B, an adaptor-less protein and SHP-1, an enzyme containing SH2 domains. We identified 5 specific amino acids that are different in the catalytic domain of the SHP-1, compared to the PTP1B, and mutated the catalytic domain of the PTP1B to reflect these differences. Enzyme activity was analyzed using self-assembled monolayer assisted MALDI mass spectrometry (SAMDI) on a library of 361 peptides containing a phosphorylated tyrosine. The peptide library allowed changes in kinetic rates and alterations in substrate specificity to be analyzed. Overall, this work illustrates the evolutionary relationship between catalytic activity and adaptor domains.

### **AEI 4**

## Protein dielectrophoresis probed with insulator based devices under DC and AC conditions

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Dielectrophoresis (DEP) occurs when polarized particles in a non-uniform electric field move towards (positive DEP) or away (negative DEP) from high electric field gradients. When applied to biomolecules, DEP has great potential as a bioanalytical tool for pre-concentration, fractionation, and separation. However, in contrast to well-characterized biological cells, the mechanism of protein DEP is not well understood limiting its potential for bioanalytical applications. The use of insulator posts (i-DEP) is a novel method that generates inhomogenous electric field gradients within a microchannel. In order to enhance the DEP force on proteins, we combine optical lithography with focused ion beam milling (FIBM) to build an array of nanostructured insulator posts in a microfluidic channel and study the DEP behavior of immunoglobulin G (IgG) molecules under DC and AC conditions. Under DC conditions, IgG molecules move according to positive DEP as reported previously [1]; however, utilizing AC, we observed a change from positive to negative DEP. Our preliminary results show that at 1Hz, IgG molecules concentrate in regions of high electric field gradients indicating positive DEP, however above 5Hz, the particles move away of these regions showing negative DEP behavior. This study indicates that such a novel fabrication process has the potential to improve applications for dielectrophoretic separation, concentration, and fractionation of biomolecules.

[1] Nakano A.; Chao T.-C.; Camacho-Alanis F., Ros A. Immunoglobulin G and bovine serum albumin streaming dielectrophoresis in a microfluidic device. *Electrophoresis* 2011, 32, 2314-2322.

## AEI 5

### Characterizing Lauryl acrylate porous polymer monoliths using HPLC

**Charlisa R Daniels<sup>1</sup>**, *cdaniels@trinity.edu*, **Nicholas J Kuklinski<sup>2</sup>**, **Brady Iba<sup>1</sup>**, **Michelle Bushey<sup>1</sup>**. (1) *Department of Chemistry, Trinity University, San Antonio, TX 78212, United States* (2) *Department of Chemistry, Furman University, Greenville, SC 29613, United States*

Fundamental characteristics of Lauryl Acrylate Porous Polymer Monoliths (PPMs) were investigated using High Pressure Liquid Chromatography (HPLC). Previous studies utilized Capillary Electrophoresis (CEC) to successfully measure the thermodynamic characteristics of these PPMs. However, CEC uses electroosmotic flow (EOF) to transport the mobile phase through the column, leaving the experiments without an accurate volume measurement. Volumetric properties of the mobile and stationary phases of the column require a more precise value of the flow rate to

measure these properties. A nano-flow HPLC was used to measure the column efficiency properties, including porosity and phase ratio of these columns. Porosity is a measurement of the void spaces in a material; therefore it is used to quantify the free space in our PPMs. The total, external, and internal porosities were measured in the presence and absence of EOF modifiers. Our data supports that despite the presence of these organic EOF modifiers, the internal porosity of our PPMs was found to be significantly less than traditional monoliths found in the literature. The phase ratio is the ratio of the volume of stationary phase to the volume of mobile phase in the column and was found to be  $0.189 \pm 0.002$  on a typical Lauryl Acrylate PPM column. With a nano-flow HPLC, the properties of Lauryl Acrylate Porous Polymer Monoliths are characterized and found to be different from traditional stationary phases.

## AEI 6

### **Development of bioanalytical platforms using original substrates such as modified optical fiber bundles or patterned paper for applications in diagnostics**

**Frederique T Deiss**, *deiss@ualberta.ca. Department of Chemistry and Alberta Glycomics Centre, Present address: University of Alberta, Edmonton, AB T6G 2G2, Canada*

This presentation will display a panel of bioanalytical devices resulting developed through my work at the interface Chemistry-Physics-Biology in different research groups: (i) Microbiological paper-based platforms in Derda group, University of Alberta, Canada; (ii) Electrochemical paper-based devices in Whitesides group, Harvard University, USA; (iii) Optoelectrochemical sensor arrays (PhD projects) under Sojic supervision, University of Bordeaux, France.

These latter high-density biosensing platforms were fabricated by nanostructuring one face of coherent optical fiber bundles using chemical etching, and functionalizing them with biological probes. One fluorescent DNA nanosensor array, where DNA probes were immobilized by electrodeposition of a polypyrrole, enabled the detection of the hybridization remotely through the imaging fiber.[1] We addressed different DNA sequences onto the same nanostructured array using electrochemical cantilevers.[2] The second opto-electrochemical biochip was a multiplexed sandwich immunoassay detected by electrochimiluminescent imaging resolved at the single bead level, a readout technique we optimized.[3] Both optical-fiber-based platforms demonstrate the potency of combining multiple physical and chemical techniques to obtain biochips with high-density and high-multiplexing potentials.

At the other end of the spectrum of diagnostic devices, we can find portable, low-cost, simple and user-friendly platforms that will permit efficient and convenient analysis at the point-of-care. Electrochemical Microfluidic Paper-based Analytical Devices (E $\mu$ PAD) used with commercial glucometer as a reader were developed for this purpose by wax-patterning and stencil-printing on paper. We demonstrated their application to quantify various analytes (e.g., glucose, lactate, cholesterol) in blood samples.[4]

Examples of paper-based platforms for high-throughput testing of soluble compounds on cell cultures, and diagnostics using microorganisms (bacteria and bacteriophage) will also be presented.

[1] Deiss, F. et al. *Analyst*, 2011, 136, 327-331

[2] Descamps, E. et al. *Lab Chip* 2013, accepted, DOI: 10.1039/C3LC50335F

[3] Deiss, F. et al. *J. Am. Chem. Soc.* 2009, 131, 6088-6089

[4] Nie, Z. et al. *Lab Chip* 2010, 10, 3163-3169

## AEI 7

### **Nitrates in the environment: Using the analytical chemistry laboratory course as a testing laboratory for an environmental chemistry class**

**Leonard Demoranville**, *leonard.demoranville@centre.edu*, *Daniel Scott, Preston Miles. Chemistry Program, Centre College, Danville, KY 40422, United States*

Students in an analytical chemistry laboratory analyzed samples of local stream water collected by students in an environmental chemistry course. Since the environmental chemistry course did not have a laboratory component, the students in the analytical course acted as a contract testing lab. The analytical chemistry students were provided with the EPA protocol for nitrate determination and were instructed to use two standard methods, ion selective electrode and UV spectroscopy, for analysis. The pooled class data were analyzed by each individual using statistical techniques that had been covered in lecture. This complex data set provided an exercise with no explicitly correct answer. This method provided students with authentic challenges faced by analytical chemists. All data were provided to the environmental chemistry students for discussions appropriate to that course. Student feedback on the activity suggested the authentic application of the theory presented in the class provided an important framework for the material.

## AEI 8

### **Single nanomaterial dynamics and imaging of gold spheres and plates**

**Mary Sajini Devadas**, *mdevadas@nd.edu*, *Todd A. Major, Zhongming Li, Shun Shang Lo, Gregory V. Hartland. University of Notre Dame, Notre Dame, Indiana 46556, United States*

Single-nanomaterial spectroscopic (SNS) techniques are widely used to investigate many physical, chemical, and biophysical phenomena which cannot be accurately determined by ensemble measurements. The merit of SNS is that it overcomes the disadvantage of sample polydispersity, which often masks important dynamical

processes. My current research entails the synthesis and the study of the ultrafast dynamics of single metal nanoparticles with different local environments using transient absorption microscopy (TA). This is done to determine the damping rates of the acoustic vibrations in single gold nanoparticles which relates to time scales at which energy dissipates to the environment. This work requires the combination of Spatial Modulation Spectroscopy (SMS) to determine the size of the Au nanoparticle optically, with correlated transient absorption measurements on the individual nanoparticle. To optimize the set-up and achieve shot-noise limited detection the laser was modulated using an acousto optic deflector (AOD) or a galvo mirror (GM). Another project in which I am involved deals with the probing of propagation lengths of surface plasmon polaritons (SPPs), in chemically synthesized gold nanoplates. This 2D material is useful for the creation of optical devices with nanoscale dimensions that guide electromagnetic energy with a lateral mode confinement below the diffraction limit of light. In this work single crystalline, micrometer-sized plates are formed by using a modified polyol protocol. Their physical dimensions were measured using Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). The synthesis, characterization, growth mechanism and SPP propagation studies will be presented along with results from SMS and TA measurements.

## AEI 9

### **Photochemistry of chromophore/transparent conductive oxide interfaces measured using transient absorbance spectroscopy in attenuated total reflectance geometry**

***Judith L Jenkins, judyj@email.arizona.edu, Mario Malfavon, Edgardo M Hernandez, Neal R Armstrong, Dominic V McGrath, S Scott Saavedra. Department of Chemistry and Biochemistry, The University of Arizona, Tucson, AZ 85721, United States***

Fast charge transfer across dissimilar organic-organic, organic-inorganic, and organic-metal oxide interfaces is critical for high photoconversion efficiency in thin film solar energy conversion platforms. Charge transfer, charge separation, and charge collection all compete kinetically with detrimental relaxation and recombination processes. However the rates of these interfacial processes are hard to predict and must be measured as novel chromophores and transparent conductive oxides (TCO) are developed. Transmission transient absorbance spectroscopy has been used to examine the photochemical kinetics of multilayer films where molecule-molecule and molecule-substrate processes occur simultaneously, but this geometry does not afford the sensitivity necessary to probe sub-monolayer chromophore films where interface processes can be isolated. In this work, transient absorbance spectroscopy in attenuated total reflectance geometry was used to monitor excited state kinetics of semiconducting nanocrystals and porphyrin-perylene diimide dyads on TCO substrates and on insulating substrates. Differences in the chromophores' excited state decay rates and ground state recovery rates as a function of the underlying substrate were used to quantitatively compare the desired interfacial charge transfer processes to the competing relaxation processes. The excited state kinetics were correlated to the

chemical and physical properties of both the chromophores and the TCOs, providing chemical rationale for the design of future active layer/TCO interfaces with sufficiently fast charge collection rates.

## AEI 10

### Optimization of nicotine analysis using solid phase microextraction

**Tina Rainey**, *clrainey@iupui.edu*, **John V Goodpaster**.*Department of Chemistry and Chemical Biology, Indiana University Purdue University Indianapolis, Indianapolis, IN 46202, United States*

A gas chromatography-mass spectrometry (GC-MS) method to analyze nicotine and its metabolite, cotinine, has been developed and optimized utilizing solid phase microextraction (SPME) of hair extractions in various solvents. There are many parameters that must be optimized in developing a SPME method, including SPME fiber type, incubation temperature, incubation time, extraction time, desorption time, and sample volume. Using a statistical experimental design is the best way to determine the optimal parameters without performing every possible parameter combination, or a “vary one parameter at a time” method. This presentation will focus on the optimization of a SPME method utilizing a central composite response surface design.

## AEI 11

### Using nonlinear optical spectroscopies to elucidate surface adsorption and reaction in systems ranging from atmospheric aerosols to drug-membrane interactions

**Grace Y Stokes**, *gystokes@chem.utah.edu*.*Department of Chemistry, University of Utah, Salt Lake City, UT 84112, United States*

Using the surface-specific vibrational spectroscopy, sum frequency generation (SFG), interactions between ozone and organic-coated mineral dust surfaces were monitored. Using an organosilane system which allows for molecular control of the orientation and steric accessibility of the carbon-carbon double bonds in surface-bound olefins, we measured the reaction rates of a wide range of terpenes and determined reactivity trends for immobilized chiral and achiral organic compounds.

Counter-propagating second harmonic generation (SHG) was used to quantify the binding of selective estrogen receptor modulators (SERMs) to model cell membranes composed of planar-supported lipid bilayers. The effects of lipid phase and order, cholesterol content, and drug charge on binding were quantified. Comparisons of SERM binding in the presence and absence of the peripheral estrogen receptor, ER<sub>A</sub>, incorporated in the lipid bilayer were also made.

## AEI 12

## Interfacial processes in Li ion batteries

**Hadi Tavassol**, [tavasso2@illinois.edu](mailto:tavasso2@illinois.edu).*Chemistry, University of Illinois Urbana Champaign, Urbana, IL 61801, United States*

My research involves characterization and control of the advanced electrochemical system presented by the modern Li ion battery. Electrochemical quartz crystal microbalance (EQCM) measurements show that substantial mass is retained on Au electrodes, while much less is retained on Sn. Matrix assisted laser desorption ionization (MALDI)-time of flight (TOF) mass spectrometry analysis of both Sn and Au surfaces after emersion of cycled electrode surfaces, shows regular repeat patterns, which confirm the presence of high molecular weight oligomerized species as a part of solid electrolyte interphase (SEI). Nature of the formed SEI and degree of oligomerization can be controlled by using electrolyte additives such as vinylene carbonate and Vinyl ethylene carbonate.

Mechanical degradation from cumulative stresses arising during cycling of electrodes and the dynamics of SEI formation are key factors in capacity retention, and battery performance. Potential dependent surface stress and strain measurements provide a quantitative and qualitative measure of the coverage dependent mechanical changes of the electrode materials during SEI formation and Li deposition particularly for advance anodes such as those made from Si, Sn, and bimetallic alloys. Electrochemical surface stress measurements on a model anode material shows that surface stress changes are determined both by the degree of lithiation and SEI evolution. While Li deposition is accompanied by compressive stress as expected, residual tensile stress is observed upon delithiation, the origin of which is the SEI which forms on the surface just as delithiation is initiated. In contrast, Sn based anodes, depending on their  $\text{SnO}_x$  content, exhibit significant changes in compressive and tensile surface stress even before Li insertion. These features occur in potential regions where there is no major interaction between Li and Sn.

Ultimately this research investigates the interplay between SEI, battery mechanical properties, and performance.

## AEI 13

### Innovative strategies for coupling separations with MALDI mass spectrometry

**Stephen J Hattan**, [shattan64@netzero.net](mailto:shattan64@netzero.net).*SimulTof Systems, Sudbury, MA 01776, United States*

The research presented here highlights projects focused on innovative means of analyzing complex biological samples. A common thread amongst the projects is to improve means for effectively and efficiently coupling of sample preparations and separations with mass spectrometry. The ability to accurately inventory and quantify the potentially 100s to 1000s of proteins that compose a given biological system often

remains a challenge to bio-analytical science. Generally, the biggest obstacles to success are sample complexity coupled with a wide dynamic range of component concentration. Often, large-scale proteomic experiments must rely on separation science to distribute and concentrate the components prior to their sequentially detection. Without separation, the capability of mass spectrometers to distinguish the various components would be overwhelmed and rendered incomplete. Regardless, in many proteomic workflows, there remains a disconnection between optimization in sample preparations and separations and sample detection by mass spectrometry. The research outline here addresses this issue directly by targeting the construction of novel substrates (sample plates and membranes) designed to capture and concentrate biological analytes after separation, preserving the resolution gained, while acting as substrates for further sample processing (e.g., protein digestion, chemical modification). Additionally, many of sample substrates are uniquely designed to interface directly with the mass spectrometer.

The applications for these novel sample plates and membranes have focused on linking protein separations or “top-down” proteomic schemes with mass spectrometry. Examples of these separations are gel-electrophoresis, isoelectric focusing, and protein chromatography. The “top-down” approach was targeted because it offers the best means for dealing with the wide dynamic range in concentration characteristic of biological samples (blood serum  $\sim 10^{12}$ ). Additionally, maintaining the protein structure helps preserve protein iso-form and glyco-form information; characteristics that may imply disease. In addition, innovative substrates designed to improve tissue-imaging analyses by MALDI mass spectrometry will also be presented.

## AEI 14

### **Spectroelectrochemical studies utilizing carbon optically transparent electrodes (C-OTEs)**

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Carbon optically transparent electrodes (C-OTEs) are a stable and efficient spectroelectrochemical platform for detailed study of electrochemical processes and interfaces. This poster displays two examples of C-OTEs based on pyrolyzed photoresist films (PPFs) as improved platforms for studying electrochemical systems. We have utilized these electrodes for oxidative-reductive electrogenerated chemiluminescence (ECL) that display a low oxidation potential for co-reactant ECL as the hydrophobic electrode surface facilitates adsorption of coreactants to generate intense ECL. Furthermore, the PPF generated C-OTEs exhibit wide electrochemical windows of stability and high optical transparency in the UV region (> 35% transmittance over 190-400 nm, and 45-61% for 400-1000 nm for the thinnest C-OTEs of 11 nm thickness). The C-OTEs perform favorably versus ITO in both oxidative-

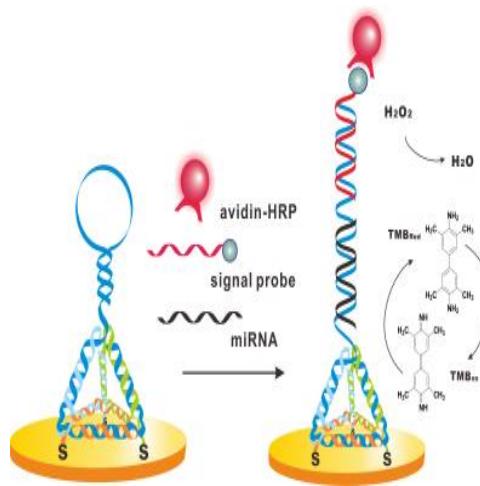
reductive and reductive-oxidative ECL studies, and are observed to be more stable in both acidic and alkaline solutions. We demonstrate how C-OTEs can be used to study the formation of electrogenerated graphitic oxides (EGO) using a combined UV-Vis spectroelectrochemical approach. Monitoring the  $\pi$ - $\pi^*$  aromatic carbon transition for reduced graphene oxide (rGO) at 270 nm and graphene oxide at 230 nm, we follow the growth of GO in KCl upon applying oxidizing potentials. X-ray photoelectron spectroscopy (XPS) and time of flight secondary ion mass spectroscopy (TOF-SIMS) are used to confirm sample composition and location of salt ions within the electrode. Formation of EGO is stable enough to be observed by UV-Vis and a new mechanism is established that is unique to alkali chloride supporting electrolytes due to formation of a solid-electrolyte interphase (SEI) which incorporates the alkali cation to stabilize the negatively charged oxygen functional groups while the presence of chloride anion acts as a passivation agent that protects the electrode surface from dissolution. This spectroelectrochemical approach highlights the detection and study of electrochemical processes that cannot be detected by electrochemical measurements alone.

## AEI 15

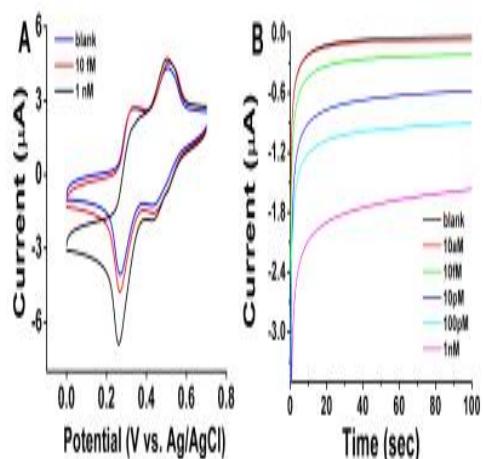
### Highly sensitive miRNA analysis using stem-loop probes carried by tetrahedron DNA nanostructures

**Gang Liu<sup>1</sup>, liug@simt.com.cn, YanLi Wen<sup>1</sup>, Li Xu<sup>1</sup>, Lanying Li<sup>1</sup>, Chunhai Fan<sup>2</sup>, Shiping Song<sup>2</sup>, Shuzhen Ren<sup>1</sup>, Ziying Zou<sup>1</sup>.** (1) *Department of chemistry, Shanghai institute of measurement and testing technology, Shanghai, Shanghai 201203, China* (2) *Laboratory of Physical Biology, Shanghai institute of applied physics, Chinese Academy of Science., Shanghai, Shanghai 201800, China*

Analysis of microRNAs (miRNAs) has attracted tremendous research interest. We here constructed a 3-D stem-loop miRNA biosensor by connecting a hairpin probe onto a tetrahedron DNA nanostructure with 3 sulfur. The DNA nanostructure improved the spatial control and accessibility of the probes. As demonstrated in Figure 1. Initially, the stem-loop probe was in “closed” state, hindering the end of the probe from being approached by the signal probes (SP). Target hybridization would break the stem duplex and exposed the probes to the SPs. Then an avidin-HRP was captured and lead to a significantly catalyzed current signal. Analysis results of miR-141 are showed in figure 2.



**Figure 1** , Scheme of the 3-D stem-loop biosensor for miRNA analysis.



**Figure 2** , A) CV curves of the 3-D stem-loop biosensor with blank, 10 fM and 1nM target miRNA (miR-141). Scan rate: 100 mV/s.; B) I-t curves for detection of miR-141 with concentrations of 0, 10 aM, 10 fM, 10 pM, 100 pM and 1 nM.

AEI 16

**Stereo specificity and mechanism of methyl group epimerization of the keto-reductase domain of the erythromycin polyketide synthase**

**Ashish Garg**, *ashish\_garg@brown.edu*, *David E Cane. Chemistry, Brown University, Providence, Rhode Island 02912, United States*

The 6-deoxyerythronolide synthase (DEBS) from *Saccharopolyspora erythraea* which by far is the most thoroughly studied modular PKS, is responsible for the biosynthesis of 6-deoxyerythronolide (6-dEB), the aglycone precursor of the antibiotic erythromycin A. The Ketoreductase (KR) domain of module 1 of the 6-deoxyerythronolide B synthase (DEBS) has been shown to catalyze an epimerization of D-2-methyl-3-ketoacyl-ACP intermediates prior to diastereoselective reduction. Incubation of recombinant KR1 with chemo enzymatically prepared (2S, 3R)-2-methyl-3-hydroxypentanoyl-ACP in the presence of NADP in D<sub>2</sub>O gave the oxidation product L-methyl-(2S)-2-methyl-3-ketopentanoyl-ACP1. This transiently generated intermediate should undergo reversible KR1-catalyzed exchange/epimerization, with incorporation of 2H at C-2. While the (2R)-[2-2H]-2-methyl-3-ketopentanoyl-ACP1 will not be reduced by DEBS KR1, back reduction of the resulting [2-2H]- 2-methyl-3- ketopentanoyl-ACP will give [2-2H]-2-methyl-3-ketoacyl-ACP1 , as a consequence of the KR1-catalyzed equilibrium isotope exchange. Our results establish definitively that the DEBS KR1 domain catalyzes a methyl epimerization during erythromycin biosynthesis.

## AEI 17

### Exploring alternate modes of Hsp90 inhibition with peptides

**Jason Gavenonis**, *jason.gavenonis@tufts.edu*, *Joshua A Kritzer*.*Department of Chemistry, Tufts University, Medford, MA 02155, United States*

Hsp90 (heat shock protein 90) is a ubiquitous chaperone protein that has been extensively studied as a target for new cancer therapies. The majority of Hsp90 inhibitors are small molecules that target the ATP-binding pocket in the protein's N-terminal domain. To discover complementary modes of Hsp90 inhibition, we used Hsp90 crystal structures to design peptide-based inhibitors that could mimic surfaces involved in Hsp90's protein-protein interactions. From these, a peptide inhibiting Hsp90 at the C-terminus was found to have 20-fold greater potency than the known small-molecule C-terminal inhibitor novobiocin, and the manner in which it inhibits the Hsp90 chaperone cycle was further elucidated through cell culture and pull-down assays.

## AEI 18

### Solution structures and models describing the thioredoxin system from *Mycobacterium tuberculosis*

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*Mycobacterium tuberculosis* (*M. tb*) resists oxidative killing in part by using the thioredoxin (Trx) system.<sup>1</sup> Trx catalyzes thiol-disulfide exchange reactions using redox

active cysteine thiols to reduce disulfides of other essential proteins.<sup>2-4</sup> Oxidized Trx is then reduced by thioredoxin reductase (TrxR) in an NADPH dependant reaction.<sup>5</sup> The *M. tb* Trx system consists of three Trx's (TrxA, TrxB, and TrxC) and one Trx reductase (TrxR). TrxR is essential for survival. TrxB and TrxC are known substrates of TrxR.<sup>1</sup> TrxA, meanwhile, has been reported to not bind to TrxR and to possibly be "cryptic."<sup>1</sup> The *M. tb* Trx system is dissimilar to the human Trx system such that inhibitor specificity for the *M. tb* Trx system should be obtainable. Thus, the *M. tb* Trx system appears to be a viable drug target.<sup>6</sup>

The objective of this study was to structurally characterize oxidized and reduced Trx's. Solution structures have been calculated using standard NMR solution experiments.<sup>7</sup> Our studies indicate that TrxA is well-folded in both oxidized and reduced states. Structures of the individual Trx's and binding models of the TrxN(N=A, B, or C)-TrxR, constructed from NMR titrations of each <sup>15</sup>N enriched TrxN and unlabeled TrxR, are discussed.<sup>7</sup> These binding models show an empty pocket between the Trx and the TrxR, that is targeted for structure-based design of uncompetitive inhibitors.

1. Akif, M., et. al. *J. Bacteriol.* **2008**, 190, 7087-7095.
2. Gleason, F. K., et. al. *FEMS Microbiol. Lett.* **1988**, 54, 271-297.
3. Ortenberg, R., et. al. *Proc. Natl. Acad. Sci. U. S. A.* **2004**, 101, 7439-7444.
4. Powis, G., et. al. *Pharmacol. Ther.* **1995**, 68, 149-173.
5. Williams, C. H., et. al. *Eur. J. Biochem.* **2000**, 267, 6110-6117.
6. Zhang, Z., et. al. *Arch. Biochem. Biophys.* **1999**, 363, 19-26.
7. Olson, A.L., et. al. *Proteins: Struct., Funct., Bioinf.* **2013**, 81, 675-689.

## AEI 19

### Modulation of nuclear receptor function at multiple levels: Agonist and antagonist ligands, receptor subtype-selective ligands, selective receptor modulators, and modulators of receptor coregulators

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Nuclear receptors such as estrogen receptor (ER) and androgen receptor (AR) are ligand-inducible transcription factors that regulate many biological functions and the misregulation of them can result in a variety of diseases such as cancer and inflammatory diseases. Therefore, the identification of small molecules that are capable

of activating or repressing particular functions of the receptors is of great interest. We have employed two methods for regulating nuclear receptor function: direct activation or inhibition of the receptors, and inhibition of a coregulatory enzyme, lysine specific demethylase 1 (LSD1), that we have identified as important for ER function. Through these studies compounds that have strong anti-inflammatory activity through the estrogen receptors but do not stimulate the reproductive system, compounds with activity in animal models of multiple sclerosis, and compounds having strong inhibitory effects in androgen receptor signaling have been identified.

## AEI 20

### **Cyclic peptides: Powerful chemical tools to elucidate biological pathways**

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There is a constant demand for new and improved chemical tools to study biological processes. Peptides represent an attractive approach for the generation of such tools, as they can mimic native protein interactions, exhibit low toxicity, and provide higher specificities and binding affinities relative to small molecules due to extensive number of interactions with their target. These properties are especially important when chemical tools are being converted into drug leads. This poster will describe research broadly focused on the design and application of cyclic peptides as chemical tools to study a range of clinically relevant targets. First, I will outline the use of cyclic peptides to enhance the pharmacological properties and stabilize the bioactive conformation of a Protein Kinase B (PKB/Akt) peptide inhibitor. These studies resulted in a 10-fold more potent, metabolically stable cyclic analog that can be used as a potential anti-cancer drug lead. Second, I will describe our efforts to probe the SAR and design non-native analogs of a cyclic peptide signal used by *Staphylococcus aureus* for quorum sensing and virulence control. These studies resulted in the discovery of a potent peptide inhibitor that attenuates virulence in this deadly pathogen at picomolar concentrations. Finally, my research goals for the Tal-Gan research lab will be discussed. These broad goals include the development of efficient synthetic pathways for cyclic peptide construction and the application of these methods to the characterization and treatment of various disease states using state-of-the-art chemistry and biological screening techniques.

## AEI 21

### **Biophysical studies on the importance of the synergistic anion in iron binding and release by ferric binding protein (FbpA)**

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Ferric binding protein (FbpA) is a member of the transferrin superfamily of proteins that binds and transports the essential nutrient iron across the periplasm in Gram-negative bacteria. Tight sequestration of iron by FbpA requires a synergistic anion. The identity of the synergistic anion depends on the environment and metabolic activity of the bacteria and several anions have been found to serve this function. We have applied spectroscopic, thermodynamic and kinetic methods in the characterization of  $\text{Fe}^{3+}$  binding and release by FbpA in the presence of various synergistic anions. These data are interpreted in the context of *in silico* modeling and biological data to develop a picture of the transport of iron into the cytoplasm of selected Gram negative bacteria.

## **AEI 22**

### **Applying NMR based metabolomic methods to study quorum sensing in microbes**

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The behavior of microbes is regulated by many effecting factors from themselves and environment. Among those factors, small molecules are always employed to stimulate or inhibit the expression of specific genes' expression.

Quorum-sensing is a mechanism, which bacteria produce and secrete cell density dependent small molecules to regulate their gene expression related to symbiosis, virulence, competence, conjugation, antibiotic production, motility, sporulation, and biofilm formation. We are using NMR based metaolomic methods combining with LC-MS to map the changes of small molecules' following quorum-sensing assays.

Microbes' metabolomic footprints are varied under different quorum-sensing conditions. We already proved that quorum-sensing up regulates the production of one group of small molecules. In the mean time, it also inhibits the production of another group of small molecules under laboratorial conditions. We are now investigating the unique small molecules under given growing conditions from several selected pathogenic microbes. We also examine these ubiquitous compounds' biosynthetic pathway, functions and receptors in the microbes and wish to apply the results for designing of new generation antimicrobial drug candidates.

## **AEI 23**

## From the bench to the blackboard

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Producing an educated, informed public is an important goal for colleges and universities. Consequently, we are developing a program to incorporate research-inspired experiments into the general chemistry laboratory, in hopes of increasing students' awareness of research and shifting their attitudes toward research in a positive direction. This poster will describe two new laboratory experiments for second-semester general chemistry, inspired by ongoing research in our own chemistry department. To address the concepts of basic organic chemistry and intermolecular forces, students synthesize and analyze cationic gemini surfactants; this experiment is derived from anionic gemini surfactant research in the department. The second experiment draws from research exploring the environmental fate of nanomaterials. The students study the kinetic properties of an oxidation reaction, in the context of initial reaction rates, under conditions similar to those reported by the researchers.

Assessing the impacts of these curricular changes in the context of our interest in students' awareness of and attitudes toward research requires a valid, reliable survey instrument. Surprisingly, no such instrument exists in the literature, despite the prevalence of surveys for measuring students' attitudes toward science in general and particular fields like chemistry, as well as instruments that probe students' views on the nature of science. Therefore, we have developed our own instrument. This poster will also discuss the iterative process of instrument design and data analysis, including evidence of validity and reliability.

## AEI 24

### Design and development of assessment instruments for health science chemistry courses

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<h2>This presentation is a compilation of several projects, some of them are still works in progress. The inventories are specifically designed for the allied-health majors. The rationale of the work, the psychometric analysis of the data, and the results will be presented.</h2><h2>The design and psychometric analysis of a GOB Concept Inventory: The General, Organic, and Biological Chemistry Concept Inventory (GOB CCI) is a multiple-choice instrument designed to assess students' conceptual understanding of the main chemistry concepts identified as essential in clinical nursing practice. This presentation will describe the development process of the individual items along with an evaluation of the pilot versions of the instrument.</h2>

*Survey of student's ability to transfer knowledge of organic chemistry to metabolic pathways:* Organic chemistry is a prerequisite for biochemistry. Students majoring in nutrition, biology, chemistry, and biochemistry were presented with several tasks pertinent to organic chemistry and their equivalent in biochemistry. The research will present the survey, the statistical analysis of students' ability to transfer knowledge between the two types of chemistry, discussions and implications of the results.

*Metabolism questioner:* Students entering into biochemistry courses with incorrect ideas regarding different metabolic pathways and bioenergetics. The interviews with the students showed some of these ideas are inherited from previous science classes. The instrument will help the biochemistry instructors to identify and consequently address students ideas.

#### **AEI 25**

#### **Next generation nanomaterial composites based on “magic sized” semiconductor nanoclusters with uniform size and core composition**

**Sukanta Dolai**, *sdolai@iupui.edu. Department of Chemistry and Chemical Biology, Indiana University Purdue University Indianapolis, Indianapolis, Indiana 46202, United States*

Development of materials composed of semiconductor nanoclusters with uniform size and core composition is a current challenge in nanotechnology. While it is very difficult to control the size and core composition for large clusters it might be practical for ultra-small clusters, as they tend to adopt a handful of structures having exceptionally high stability. These thermodynamically stable ensembles of atoms are often called “magic sizes” and are formed by closed shells of atoms providing uniformity in their chemical composition approaching that of small molecules. Introduction of semiconductor nanoclusters having uniform core composition into the currently available devices would improve performance. The key requirements for achieving these include developing new synthetic methods, understanding principles governing formation of “magic sized” nanoclusters, and preparation of novel nanomaterial composites. More specifically, I plan to focus my research on (1) synthesis of “magic sized” semiconductor nanoclusters of various functionalities with uniform size and core composition via colloidal approach (2) production of novel nanocomposites based on conducting polymers and semiconductor nanoclusters, (3) developing strategies to control their long and short range interaction (4) electronic band gap detection through electrochemical methods. These will generate novel nanomaterials for the advancement of lasers, LEDs, photovoltaic devices and electrocatalysts.

#### **AEI 26**

#### **Single-pot synthesis of uniform glucan multilayers on oxide particles**

**Joseph Jankolovits**, [jankolovits@berkeley.edu](mailto:jankolovits@berkeley.edu), Oz M. Gazit, Michael M. Nigra, Alexander Katz. *Department of Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA 94720-1460, United States*

Polymer coatings are used widely to tune the surface chemistry of solids in biomaterials, paints, and other materials. Covalently grafted polymer coatings provide advantageous stability, though their prevailing syntheses involve multiple step procedures, low solid yields, low surface coverage, and/or non-uniformity on the nanoscale. This poster presents a novel method for uniformly grafting polymer multilayers on inorganic oxide particles in a single-pot process. Implications of this coating for the stabilization of paint pigment dispersions and nanomedicine will be discussed.

## AEI 27

### **Biomimetic and microfluidic approaches to biomolecular function and application**

**Sarah L. Perry**, [perrys@uchicago.edu](mailto:perrys@uchicago.edu). *Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637, United States*

Living cells have evolved sophisticated intracellular organization strategies that are challenging to reproduce synthetically. Biomolecular function depends on both structure and the properties of the surrounding medium. The ability to correlate structure to function at biologically relevant timescales, simulate the *in vivo* environment, and isolate biological networks for study in an artificial milieu represent engineering challenges with tremendous potential to impact both biological studies and biomedical applications.

Efforts to understand biomolecular structure-function relationships have relied heavily on static structural depictions that do not fully describe the dynamic nature of reaction processes. This limitation is the result of difficulties in applying dynamic or time-resolved crystallographic methods to a majority of biomolecular targets. These challenges are associated with radiation damage and/or simultaneous and repetitive triggering of the biomolecular reaction within a crystal. X-ray transparent microfluidic platforms for protein crystallization can be used to address these challenges, enabling multi-crystal serial analysis strategies to avoid both radiation damage and the necessity of repeatedly cycling a reaction. Such chips can also enable high throughput structural analysis with respect to many variables including pH and ionic strength to better understand biomolecule function.

The challenge in designing synthetic organelles and *in vivo* microenvironments is maintaining crowding and compartmentalization while controlling the available intermolecular interactions. Emerging experience has shown that complex coacervates (liquid-liquid phase separation) utilizing biomolecules produces an effective biomimetic microenvironment. Initial efforts are focused on understanding how functionalities, introduced through sequence-specific motifs, affect biomolecule sequestration and function. Molecular design enables the use of structure and microphase separation as additional design parameters. Using these strategies, I propose the development of

artificial organelles for applications in biochemistry, bioenergetics, biocatalysis, and biomedicine. Insights gained from developing such systems may provide insight into the function of analogous membraneless organelles as well as potential pathways for the evolution of prebiotic life.

## AEI 28

### **Computational chemistry for nanotechnology, sustainable energy, and biological objects: From molecular dynamics of single molecules to quantum transport in interfacial systems**

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Over the course of my doctoral work I focused on development of the classical molecular dynamics methods and analytical models and applying them to complex systems and the processes taking place on the large time scales. The systems studied included a variety of the molecular machines, working as either single molecules on interfaces and in solutions or as the collective ensembles in crystalline solids. These systems are the promising building blocks which can be used in nanotechnology, electronics, for biological transport and drug-delivery. With the help of physically-motivated models for description of interactions and by using efficient propagation techniques we have been able to gain valuable insights into fundamental principles of operation of such interesting objects.

Currently, in my post-doctoral work, I am focusing on the development of the quantum dynamics methods and their application to the ultrafast processes, taking place on the picosecond and sub-picosecond timescales. Such processes occur in various photovoltaic and photocatalytic applications as well as in biological photosystems. Thus, the fundamental understanding of their mechanisms and properties is important for improving efficiency of the solar and photochemical cells and for the rational design of new photoactive materials, including those in biological systems. In particular, the projects I am currently working on include the photocatalytic water splitting on oxynitride semiconductors, singlet fission in organic solar cells, as well as the relaxation and charge transfer dynamics in a variety of condensed matter systems.

The two approaches I pursued during my Ph. D. and postdoctoral studies, described above, are complementary to each other and provide a valuable basis for the next logical step I'd like to develop in my independent career – building the physically-motivated multi-resolution models and using them to gain a fundamental understanding of the processes in nanotechnology and sustainable energy applications as well as in biological objects.

## AEI 29

### Molecular dynamics simulations of large biomolecular complexes

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Large biomolecular complexes, such as protein filaments and molecular machines, are involved in a wide array of important cellular functions. Here we present the results from recent molecular dynamics simulation studies on several such systems: the actin filament, the complex of actin and myosin (actomyosin), and the type IV pilus from *Neisseria gonorrhoeae*. Actin is a protein which forms long filaments in the cell, and is a major element of the cytoskeleton. The actin nucleotide state (whether actin is bound to ATP or ADP) can affect global properties of the filament, such as its persistence length and torsional rigidity. Additionally, actin filament dynamics can be regulated by the binding of other proteins (for example the molecular machine myosin), as well as by the presence of cations bound at specific filament sites. We carried out molecular dynamics simulations of actin filaments in the presence of either myosin or filament-bound cations to investigate the influence on filament behavior. Another large protein filament, the type IV pilus, is found to protrude from the surface of a variety of infectious bacteria. Type IV pili are known to withstand very large tension forces, and the pilus from *Neisseria gonorrhoeae* has been experimentally demonstrated to exhibit a force-induced conformational transition. Steered molecular dynamics (SMD) was used to pull on a type IV pilus filament in order to understand the nature of the interactions that contribute to the great strength of bacterial pili. The SMD simulations led to the exposure of an amino acid sequence initially buried within the filament, consistent with experimental observations. Such exposed sequences could be used as potential drug targets for mitigating bacterial infection.

## AEI 30

### Molecular recognition studied using computation and experiment

**Ryan G Coleman**, [ryan.g.coleman@gmail.com](mailto:ryan.g.coleman@gmail.com). *Department of Pharmaceutical Chemistry, University of California, San Francisco, United States*

Research in my future laboratory will involve chemical efforts towards finding new drugs for important diseases while gaining a greater understand of the theoretical processes

behind molecular recognition in the process, using a combined experimental and computational approach.

In the past I have studied the biophysical nature of druggable binding sites and algorithms for discovering them, algorithms for finding and examining binding sites and tunnels in proteins and hyperthermostable proteins. My current research focuses on molecular docking, both on the methods development side and on the experimental side. In the future, I will focus on 1) algorithms and theoretical understanding of protein-ligand interactions 2) examination and application with protein targets and small molecules and 3) collaborations with other labs interested in finding new chemical tools with desired properties for their protein targets of interest.

## **AEI 31**

### **Computational investigations into the chemistry of biomolecules and functionalized nanomaterials**

**Haining Liu, *hliu38@eng.ua.edu*. Department of Chemical and Biological Engineering, University of Alabama, Tuscaloosa, AL 35487, United States**

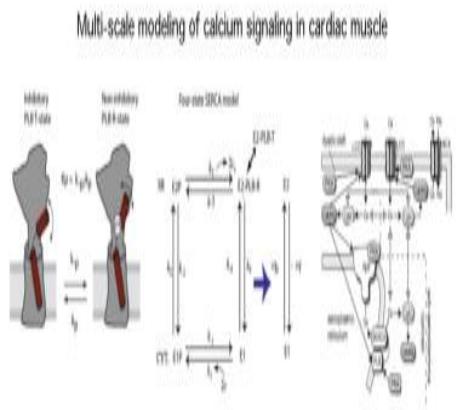
Understanding the properties of biomolecules and nanomaterials is of great interest in the scientific community. In my work, I have been using computational chemistry methods to study various biomolecules and functionalized nanomaterials. For example, the chemical mechanism of the methemoglobinemia process caused by an antimalarial drug primaquine was investigated using docking, quantum mechanics and QM/MM methods. The methemoglobinemia toxicity is a serious concern for this drug that has been unknown for more than six decades. By studying the primaquine...hemoglobin interaction and the subsequent chemistry upon such an interaction, we proposed the first mechanism in the literature to explain the methemoglobinemia caused by primaquine. In addition to biomolecules, the chemistry of various material and nanomolecules were also studied by computational methods. For example, the fundamental acid-base properties of imidazole, the precursor for a polymer membrane material to be used for CO<sub>2</sub> capture, were studied by quantum mechanics methods. The effects of various substituents were investigated and the results are able to aid the future design of this material. Furthermore, the mechanism of the formation of a gold nanoparticle was studied by quantum mechanics methods. Our results explain various experimental findings and provide insights into how this nanoparticle is formed. An overview of my other relevant work will also be presented.

## **AEI 32**

### **Multiscale modeling of calcium signaling in cardiac muscle: An atomistic- to cellular-scale perspective**

**Peter Kekenes-Huskey, *pkekeneshuskey@ucsd.edu*. Pharmacology, University of California San Diego, La Jolla, CA 92093, United States**

My highly interdisciplinary postdoctoral studies focus on multi-scale simulations of cardiac function using a combination of molecular dynamics, partial differential equations and systems biology. At the cellular level, I have devised reaction-diffusion models for analyzing calcium dynamics in microscopy-derived cardiac ventricular myocyte geometries. At the molecular scale, I have examined cardiac proteins that regulate  $\text{Ca}^{2+}$  signaling, through molecular- and Brownian dynamics simulations of the Sarcoplasmic Reticulum  $\text{Ca}^{2+}$  ATPase (SERCA) and Troponin. As electrostatic interactions and the configuration of macromolecular structures conspire to tune  $\text{Ca}^{2+}$  diffusion, I developed continuum models for predicting association kinetics and macroscale effective diffusion tensors. I have leveraged these atomistic techniques to integrate a state model of SERCA function in a subcellular model of excitation-contraction coupling.



The PubChem3D project aims to assist in the analysis of biologically similar molecules that are difficult to interrelate using traditional 2-D similarity methods. It generates a 3-D conformer model for ~92% of chemical records in PubChem. A pre-computed multi-conformer 3-D similarity search for each chemical gives immediate access to a set of structurally similar compounds in PubChem as well as their respective superpositions. The PubChem3D Structure-Activity Relationship (SAR) Cluster database helps one to discover useful bioactivity data patterns. In conjunction with the rich annotation available in PubChem, such as experimental 3-D structure, relevant patent documents, cited scientific literature, and medication information, one can quickly navigate the structurally similar compounds that share common annotations. In addition, PubChem's location at the National Center for Biotechnology Information (NCBI) allows the user to readily access integrated pertinent information beyond that found in PubMed, such as protein target, gene, disease, and pathway.

The coupling of PubChem's massive collection of chemical and bioactivity information with SAR analysis capabilities helps present new opportunities for the biomedical research community to facilitate chemical probe development and drug discovery. This presentation will provide an overview of the PubChem3D resources and demonstrate their utility for finding useful bioactivity data patterns.

#### **AEI 34**

##### **Dynamics of hot electron relaxations**

**Alex Kutana**, *kutana@rice.edu. Department of Mechanical Engineering and Materials Science, Rice University, Houston, TX 77005, United States*

Charge separation and relaxation play an important role in a variety of nonequilibrium processes. In nanocrystal-based photovoltaic cells, photoinduced charge separation enables the delivery of charge carriers to the external circuit. Understanding the microscopic details of the dynamics of electrons and holes in nanocrystals during charge separation is a prerequisite for successful design of efficient photovoltaic cells. Charge separation is effected by the scattering of carriers on phonons, and here we investigate the time-dependent phonon-induced behavior of excited electrons and holes in semiconductor nanocrystals with ab initio methods. Intrinsic and codoped Si nanocrystals are selected as model systems for studying intraband relaxations. Using density functional formalism in conjunction with the density matrix theory, we follow the microscopic details of dynamics of electrons and holes in Si quantum dots after injection. Our microscopic description allows extracting any of the observables of interest, in particular we are able to calculate relaxation times and spatial locations of the carriers.

#### **AEI 35**

##### **Allosteric regulation of protein motion and function**

**Sara E Nichols**, [senichols@ucsd.edu](mailto:senichols@ucsd.edu).*Department of Pharmacology, University of California, San Diego, La Jolla, CA 92093, United States*

The goals of my research are to characterize the modulation of protein motion and function to provide rational insight for drug discovery. A key strategy for targeting therapeutically relevant proteins is seeking ways to allosterically modulate these molecular machines. Long-range allostery involves action at a pocket, distal to the active site, which modulates the function of the protein. Identifying and characterizing these binding pockets can provide highly specific control mechanisms, particularly when the active site is conserved. Our computational toolbox includes sequence based informatics techniques coupled with complementary physics-based molecular modeling. With these tools we are motivated to identify novel chemistry and modulating mechanisms to tackle dysfunctional cell signaling pathways.

### **AEI 36**

#### **Computer aided chemistry for understanding DNA damage, catalysis, and noncovalent interactions**

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My research has over the years focused on using computational chemistry to study biologically relevant systems. This research has covered a variety of interesting topics such as catalysis, transition metal chemistry, halogen bonding, carbon based materials, and drug discovery. In this presentation, which summarizes some of my previous research, I will try to convey the strength and breadth of computational chemistry by addressing four questions and how I envision using this in my future research. The following topics will be discussed: (i) Can low energy electrons with virtually no kinetic energy damage DNA? (ii) How does the P450 enzyme direct the reaction mechanism in aromatic oxidation of dopamine? (iii) What is a halogen bond and how can we model it with a classical force field in drug discovery? (iv) Can a polarizable force field accurately describe the interface between graphene surface and water or ions?

### **AEI 37**

#### **Equilibrium solvation site analysis without simulation**

**Daniel J. Sindhikara**, [sindhikara@gmail.com](mailto:sindhikara@gmail.com).*Department of Science and Engineering, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan*

Here we derive, implement, and apply equilibrium solvation-site analysis for biomolecules. Our method utilizes 3D-RISM calculations to quickly obtain equilibrium solvent distributions without either necessity of simulation or limits of solvent sampling. Our analysis of these distributions extracts highest likelihood poses of solvent as well as entropies, enthalpies and solvation free energies. This method can be used not only for

visual analysis of active site solvation but also for virtual screening methods and experimental refinement.

## AEI 38

### Development and application of computational methods to biological and artificial systems

**Eduardo M Sproviero**<sup>1,2</sup>, *e.sproviero@usciences.edu*, *Vojislava Pophristic*<sup>1</sup>. (1) *Chemistry & Biochemistry, Usciences, Philadelphia, PA 19143, United States* (2) *Department of Chemistry, Yale University, New Haven, CT 06520, United States*

My research work has been focused in the study of macromolecules, and smaller molecules with biological interest and technological applications. Many aspects of my research were centered on systems with transition metal complexes, as they have particular computational requirements, and are important in catalysis, materials synthesis, photochemistry, and biological systems.

The methodologies that I applied in my research range from Molecular Mechanics (MM), to *ab initio*, including hybrid QM/MM methods. At the *ab initio* level, I devised methodologies to evaluate and decompose intramolecular interactions into electrostatic, polarization, charge transfer, and core repulsions. At the pure MM level, I developed force field (FF) methodologies to account for dihedral energy coupling in amide foldamers, in the context of the AMBER programs. At the QM/MM level, I collaborated in the development of the Moving-Domain QM/MM method, which allows the computation of properties of macromolecules of biological relevance, at the equivalent of a QM level.

Applications range from the interpretation of the dependence of molecular properties on conformation and molecular substituents (*ab initio*), elucidation of atomistic models of the active site of photosystem II (a membrane protein that driven by solar light, catalyzes the conversion of water into electrons, protons, and molecular oxygen), the development of computational models of biomimetic systems that convert solar energy into an electron flow, the development of FF parameters for foldamers with the aim of creating artificial oligomers that carry specific biological functions, etc.

## AEI 39

### Physics-based, computational approaches to ligand discovery and design

**Robert V Swift**, *rvswift@ucsd.edu*, *Rommie E Amaro*. *Department of Chemistry & Biochemistry, University of California, San Diego, La Jolla, California 92093-0340, United States*

Discerning the molecular basis of disease and its treatment requires a holistic understanding of the complex and dynamic processes occurring across diverse length and time scales within the cell. My research is aimed at the development and

application of cutting-edge computational, biophysical models to provide a deeper understanding of the fundamental dynamics and thermodynamics underlying these processes. Such knowledge can serve as a blueprint that guides the discovery and optimization of small molecules to serve a range of purposes, from molecular biology probes, to drugs safe for human consumption. At the interface of structural biology, chemical physics, scientific computing, and molecular pharmacology, my research goals are to: enhance the utility of virtual screening methods by integrating target flexibility and target specific scoring functions; advance rigorous, absolute and relative binding free energy estimates by including alternative ligand tautomers and receptor protonation states; improve structure-based absorption, distribution, metabolism, excretion, and toxicology (ADMET) property prediction. Following the precedence set during my postdoctoral work, I will actively cultivate collaborations with the long-range goal of contributing significantly to the discovery and design of chemical therapeutics. Importantly, my scientific goals provide the technical and intellectual challenges that nurtures student development, an objective I'm committed to.

#### **AEI 40**

#### **Catalytic processes for the production of biobased aromatics, chemicals, and petrochemicals from renewable feedstocks**

**Swapnil L. Fegade**, *swapnil.fegade@my.und.edu*. *Department of Chemical Engineering, University of North Dakota, Grand Forks, North Dakota 58202, United States*

A series of exploratory experiments were conducted to investigate the feasibility of producing variety of chemicals from crop oil. The cracking of crop oil resulted in the formation of aromatics such as benzene, toluene, ethylbenzene, and xylenes, along with short and medium chain olefins. Catalytic reforming experiments on these bio-based olefins suggested that zeolite such as ZSM-5 was the best suited catalyst for the production of aromatics. Design of experiments (DOE) methodology was used to find out which reaction conditions (factors) had significant impact on the aromatization. Crop oil could be renewable feedstocks for biofuels and chemical production and this work may contribute significantly to sustainable energy research.

#### **AEI 41**

#### **Solar energy conversion using biohybrid electrodes based on nanomaterials derived from plants**

**Gabriel LeBlanc<sup>1</sup>**, *gabriel.leblanc@Vanderbilt.Edu*, **Evan A Gizzie<sup>1</sup>**, **Darlene Gunther<sup>2</sup>**, **G. Kane Jennings<sup>2</sup>**, **David E Cliffel<sup>1</sup>**. (1) *Department of Chemistry, Vanderbilt University, Nashville, TN 37235, United States* (2) *Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, TN 37235, United States*

Photosynthesis is the process by which plants, algae, and cyanobacteria convert our most abundant energy source (solar radiation from the sun) into stored energy in the form of reduced carbon. This process has supported the energy demands of the earth since the beginning of life, and continues to fuel our ever increasing demand. As the fossil fuels that were stored by this process become increasingly difficult to extract, we must find alternative means for energy generation. Here, we present research demonstrating how the nano-materials produced by plants, specifically Photosystem I, can be extracted and utilized to modify common electrode materials. The global abundance and exceptional properties of Photosystem I make this biomaterial an ideal candidate for use in solar energy conversion devices. Our research has demonstrated how we can incorporate these biohybrid electrodes into photovoltaic devices, photoelectrochemical cells, and hydrogen generation systems.

### *Acknowledgements*

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### **AEI 42**

#### **Importance of the metal–oxide interface in catalysis: In situ studies of the water–gas shift reaction by ambient-pressure X-ray photoelectron spectroscopy**

***Kumudu Mudiyanselage, kmudi@bnl.gov, Dario Stacchiola. Department of Chemistry, Brookhaven National Laboratory, Upton, NY 11973, United States***

In situ investigations of reactions over well-defined model catalysts are essential to gain a molecular level understanding of catalytic processors. Inverse model catalysts (oxide-nanoparticles/metal-substrate configuration) show remarkable activity for many catalytic reactions such as water-gas shift, methanol synthesis, and CO oxidation. We have prepared and characterized an inverse  $\text{CeO}_x\text{-Cu}_y\text{O}/\text{Cu}(111)$  model catalyst, and studied the water-gas shift reaction (WGSR;  $\text{CO}+\text{H}_2\text{O} \rightarrow \text{H}_2+\text{CO}_2$ ) using near ambient pressure X-ray photoelectron spectroscopy (NAP-XPS), infrared reflection absorption spectroscopy (IRRAS) and density functional theory (DFT) calculations.<sup>1</sup> The most abundant surface species on  $\text{Cu}(111)$  under WGSR conditions is adsorbed CO whereas adsorbed bent carboxylate ( $\text{CO}_2^{\delta-}$ ) species are identified over  $\text{CeO}_x/\text{Cu}(111)$  with the ceria in a highly reduced state. By combining in situ experimental results with calculations, we show that the precursor for the formation of  $\text{CO}_2^{\delta-}$  is a carboxy (HOCO) intermediate on the metal-oxide interface. Even though the WGSR over  $\text{CeOx/Cu}(111)$  catalysts can occur by both redox and associative mechanisms, the study presented here shows that the presence of the oxide-metal interface activates the more efficient associative mechanism pathway and leads to an increase by more than one order of magnitude in the activity of the  $\text{CeO}_x/\text{Cu}(111)$  system relative to that of  $\text{Cu}(111)$ . The observed results also indicate that formate species are not likely to be key intermediates

in the WGSR over  $\text{CeO}_x/\text{Cu}(111)$ . Our study illustrates the power of *in situ* mechanistic studies on well-defined catalysts and the important role that metal-oxide interfaces can play in catalysis.

(1) Mudiyanselage, K.; Senanayake, S. D.; Feria, L.; Kundu, S.; Baber, A. E.; Graciani, J.; Vidal, A. B.; Agnoli, S.; Evans, J.; Chang, R.; Axnanda, S.; Liu, Z.; Sanz, J. F.; Liu, P.; Rodriguez, J. A.; Stacchiola, D. J. *Angew. Chem. Int. Ed.* **2013**, 52, 1.

## AEI 43

### **Detailed Raman and X-ray analysis of electrolyte dopants in Li-ion electrochemical cells**

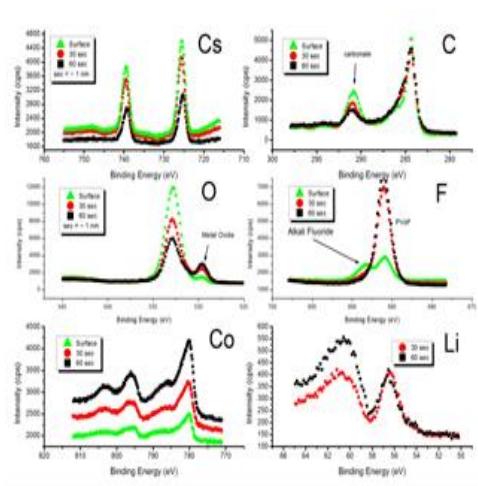
**Christopher J Patridge**<sup>1</sup>, *christopher.patridge.ctr@nrl.navy.mil*, **Corey T Love**<sup>2</sup>, **David E Ramaker**<sup>2</sup>. (1) Chemistry Division, NRC/Naval Research Laboratory, Washington, DC 20375, United States (2) Chemistry Division, Naval Research Laboratory, Washington, DC 20375, United States

#### **Introduction:**

Understanding and controlling the chemistry at the solid-electrolyte interface (SEI) in electrochemical storage devices is critical for improving safety and the projected long-term use in transportation and grid applications. In a unique approach, we have doped our electrolyte solutions ( $\sim 5 \text{ mg/mL}$ ) using larger alkali cations ( $\text{Rb}^+$ ,  $\text{Cs}^+$ ) salts. These dopants incorporate as species similar to those formed by lithium cations in the SEI.

#### **Experimental and Results:**

Half and full electrochemical cells of micro and nanoscale  $\text{LiCoO}_2$  are probed *in-situ* using micro-probe Raman spectroscopy, as well as X-ray absorption spectroscopy. Depth profiling using X-ray photoelectron



**Figure 1.** XPS depth-profiles of the  $\text{LiCoO}_2$  cathode after washing the electrode.

spectroscopy (XPS) shows changes that correlate with the Cs and Rb retained near the surface of the electroactive materials.

### Acknowledgements

The authors thank the Office of Naval Research for financial support. The synchrotron measurements were successful due to the help of Dr. Kumi Pandya. The National Synchrotron Light Source is supported by the US Department of Energy, Division of Material Sciences and Division of Chemical Sciences, under contract number DE-AC02-98CH10886. The X11 beamline is supported by the Naval Research Laboratory and contributions from Participating Research Team (PRT) members.

### AEI 44

#### Shape-controlled nanoscale materials and their applications as biological sensors

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The development of biological sensors with high selectivity and sensitivity benefits from the use of well-defined size- and shape-controlled nanoparticles. We report a facile, one pot, green synthetic process for developing size- and shape-controlled metallic and bimetallic nanomaterials, as well as studies to understand their interactions under various environmental conditions. Monodisperse metallic and bimetallic nanoparticles were fabricated at room temperature using environmentally friendly reaction conditions. These nanostructures were produced with controlled size, shape, composition, crystallinity, and structure (i.e. hollow vs. solid). Controlling the morphology of metal

nanoparticles is essential toward understanding their structure-function properties especially under varying temperature, pH and ionic strength conditions. Shape control of metal nanomaterials is important because it allows the tuning of their optical, magnetic, and catalytic properties. The synthesis of well-defined anisotropic nanoparticles under green reaction conditions is important toward advances in nanoscale synthesis. Characterization of the nanoparticles was carried out using high resolution transmission electron microscopy (HRTEM), x-ray diffraction (XRD), small angle electron diffraction (SAED) and energy dispersive spectroscopy (EDS). The use of the nanomaterials in the detection of biological contaminants will be presented.

## AEI 45

### Investigation of hydroxyl radical reactivity in a suburban environment

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The hydroxyl radical (OH) is an important atmospheric oxidant. Total OH reactivity, which is the inverse of the lifetime of OH, is an important quantity used to investigate atmospheric OH sinks. Measurements of total OH reactivity can provide information on the presence of unidentified reactive species that may be important for the formation of photochemical pollutants such as ozone.

An instrument dedicated to ambient total OH reactivity measurements, based on an adaptation of the discharge-flow technique used for radical kinetics studies, has been developed. Ambient air is sampled into a flow tube reactor where OH is continuously generated within a movable injector. This instrument monitors time-resolved decays of OH from which the total OH reactivity can be derived.

Measurements of ambient total OH reactivity and ambient concentrations of reactive trace species, which included nitrogen oxides (NOx), ozone, and speciated measurements of volatile organic compounds, were made at the Pasadena ground site

during the CalNex field campaign, which was conducted in May-June 2010. This site, due to its location downwind of emission sources in Los Angeles, presents an opportunity to examine the OH and VOC chemistry of aged air masses, whose OH reactivity has not been extensively studied. Ambient OH reactivity measurements at the Pasadena ground site will be presented and compared to the total OH reactivity calculated from collocated measurements of ambient concentrations of reactive trace species. The implications for urban OH and VOC chemistry will be discussed.

## AEI 46

### Assessing the effects of quantum dots in the terrestrial environment: Earthworm oxidative stress and uptake of cadmium

**David T.R. Stewart**<sup>1</sup>, *dts8@buffalo.edu*, **Katia Noguera-Oviedo**<sup>1</sup>, **Vincent Lee**<sup>1</sup>, **Sarbajit Banerjee**<sup>1</sup>, **David F. Watson**<sup>1</sup>, **Bryant Nelson**<sup>2</sup>, **Diana S. Aga**<sup>1</sup>. (1) *Department of Chemistry, University at Buffalo, SUNY, Buffalo, New York 14260, United States* (2) *Materials Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, MD 20899, United States*

Quantum dots are an increasingly important class of nanomaterials, but they are commonly made with toxic elements. It is not currently known if quantum dots will be as toxic to soil organisms as the ingredient metals, or if indeed they may be more toxic. One limitation in determining the nanotoxicity of engineered nanomaterials is the lack of a sensitive method to determine sub-lethal effects in test organisms. Two approaches to this problem have been utilized. First, Inductively Coupled-Plasma Mass Spectrometry was used to determine the bioaccumulation of cadmium and selenium from a very low concentration of quantum dot exposure (1 mg/kg cadmium). The results of the elemental analysis demonstrate that quantum dots would be a source of available cadmium if released into the soil and suggest that quantum dots become more available as they degrade over time. Second, a Liquid Chromatography Tandem Mass Spectrometry method to detect and quantify glucose metabolism intermediates in earthworms experiencing oxidative stress was developed. Oxidative stress is a common adverse effect observed in toxicological studies. Assessing oxidative stress can provide a more sensitive test than other currently available toxicity tests. The combination of these approaches provides a powerful toolset for assessing the effects of quantum dots, and other metallic nanoparticles, in the terrestrial environment.

## AEI 47

### Interactions at boundaries: Exploring surface area, length scales, and pore volume phenomena in nanofibrous assemblies

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Electrospinning is a facile nanofabrication technique that produces fibrous assemblies of ultra-fine fibers, 20-1000 nm in diameter, from a charged droplet of spinning solution. These fibers are continuous filaments with lengths up to several meters resulting in extraordinarily high surface to volume ratios. In essence, the majority of the fibrous material is surface or is within nanometers of the surface making electrospun nanofibers excellent candidates for applications that depend on high surface areas, local interactions, selectivity and hierarchical porosity. Two applications of these assemblies are chemical sensors fabricated from fluorescent composite polyelectrolyte complexed nanofibers and electrochemical double layer capacitor (supercapacitor) electrodes fabricated from electrospun carbide derived carbon nanofelts.

The fluorescent nanofiber sensors were electrospun from a spinning dope of Polyacrylic acid complexed with Chitosan and quantum dots. These composite fibers exhibited uniform fiber morphologies and the fluorescence peak of the quantum dot composites was unchanged. To explore the sensing applications of these nonwoven assemblies we exposed the mats to a range of pHs and changes in humidity. The mats exhibited recoverable fluorescence quenching when exposed to high humidity and demonstrated sensitivity to changes in pH. Specifically these fibers demonstrated the quantum dot inclusions were highly sensitive to the local changes in pH at the boundaries between the hydrophobic and hydrophilic regions of the polyelectrolytes in the interior of the fibers.

The second application is the use of polymer-derived ceramics to synthesize hierarchical porous carbon fibrous materials such as electrospun nanofelts. These electrodes have demonstrated excellent power handling ability leading to energy storage devices showing fast charge and discharge rates. At the same time, such fiber electrodes eliminate the need for conductive additives or organic binders used in conventional devices while remaining flexible and opening up novel applications, such as wearable electronics.

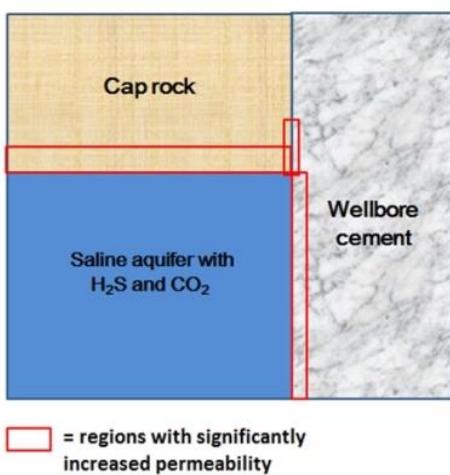
#### **AEI 48**

#### **Development of a 2D reactive transport model to predict acid gas leakage potential through cement–caprock interface under geologic sequestration conditions**

***Liwei Zhang<sup>1</sup>, zlwe88@gmail.com, Barbara G Kutchko<sup>1</sup>, Christina L Lopano<sup>1</sup>, Brian R Strazisar<sup>1</sup>, David A Dzombak<sup>2</sup>, David V Nakles<sup>2</sup>, Li Li<sup>3</sup>, Leopold Brunet<sup>3</sup>.*** (1) National Energy Technology Laboratory, Pittsburgh, PA 15236, United States (2) Civil and Environmental Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, United States (3) Department of Energy and Mineral Engineering, Penn State University, University Park, PA 16802, United States

Capture and subsurface co-sequestration of acid gas (H<sub>2</sub>S and CO<sub>2</sub>) from purification of natural gas is one approach that can reduce the emissions of CO<sub>2</sub> and H<sub>2</sub>S. To implement acid gas co-sequestration, the potential of acid gas leakage through the

interface between caprock and wellbore cement of the abandoned well needs to be evaluated, and that potential can be evaluated by assessing permeability change of caprock and wellbore cement at the interface. In this study, the permeability changes of caprock and wellbore cement exposed to acid gas at the interface were studied via model simulation using the reactive transport modeling program CrunchFlow. Two types of wellbore cement (neat class H cement and pozzolan-amended class H cement) were studied. Three types of acid gas composition (0% H<sub>2</sub>S + 100 mol% CO<sub>2</sub>, 20 mol% H<sub>2</sub>S + 80 mol% CO<sub>2</sub>, and 40 mol% H<sub>2</sub>S + 60 mol% CO<sub>2</sub>) were studied as well. Model simulation results show that after 30 years of exposure to CO<sub>2</sub> and H<sub>2</sub>S under geologic sequestration conditions (323K and 150 bar), an increase of effective permeability of wellbore cement and caprock (10<sup>4</sup> orders of magnitude) at the interface only occurred at regions very close to the storage aquifer



. As a result, the potential for acid gas leakage through caprock--wellbore cement interface was not high.

#### AEI 49

#### Half-sandwich Fe electrocatalysts for H<sub>2</sub> oxidation and production

**Tianbiao Liu**, Tianbiao.Liu@pnnl.gov. Pacific Northwest National Laboratory, Richland, WA 99354, United States

To address the rising energy demands, electrocatalysts based on inexpensive and earth-abundant metals are needed to convert renewable energy sources (e.g. solar, wind etc.) into chemical fuels (e.g. H<sub>2</sub>) and to promote the release of energy in chemical fuels as electricity. A series of half-sandwich Fe-hydride complexes, [Cp<sup>F</sup>Fe(P<sup>tBu</sup><sub>2</sub>N<sup>R</sup><sub>2</sub>)H], featuring built-in pendant amines as proton relays, have been developed as highly active molecular electrocatalysts for H<sub>2</sub> oxidation and H<sub>2</sub> production from weak acids (where Cp<sup>F</sup> represents substituted cyclopentadienide ligands and P<sup>R</sup><sub>2</sub>N<sup>R</sup><sub>2</sub> are substituted 1,5-diaza-3,7-diphosphacyclooctane ligands).

## AEI 50

### Correlations and differences between uranium(VI) arsonates and phosphonates

**Pius O. Adelani**<sup>2</sup>, *padelani@nd.edu*, Peter C. Burns<sup>1,2</sup>. (1) Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN 46556, United States (2) Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, Notre Dame, IN 46556, United States

Uranyl phosphonates have displayed rich and fascinating structural chemistry; most of the structures are layered, and the metal ions are bridged by the phosphonate moiety. The structural chemistry of metal arsonates are expected to be similar to those of the metal phosphonates, but the larger ionic radius and longer As–O bond length of As(V) compared to P(V) could greatly influence their structural and physical properties. This presentation will compare results from my current studies with arsonates to past work with phosphonates.

## AEI 51

### Metallic nanoparticles for biorenewables conversion via hydrogenation and photocatalytic reactions

**Liyana A. Wajira Ariyadasa**, *wajira.ariyadasa@wmich.edu*, Sherine O. Obare. Department of Chemistry, Western Michigan University, Kalamazoo, MI 49008, United States

There is a critical global need for renewable materials to replace crude oil as the primary feedstock for production of fuels and chemicals. The production of fuels and chemicals from biomass has received much research attention. One of the major challenges is to design robust catalysts to achieve reaction selectivity under mild conditions. Nanosized metal and metal oxide particles show unique optical, electronic, catalytic, chemical, and physical properties relative to their bulk materials. Nanoscale materials provide high surface area which facilitates exposure of the surface atoms and thus leads to improved reaction conversions. In this project, nanoscale particles have been investigated as catalysts for the conversion of biorenewable resources. Pd and TiO<sub>2</sub> nanoparticles were investigated as catalysts for hydrogenation of aldehydes and deoxygenation of carboxylic acids. Cinnamaldehyde and citral were used as model aldehydes and oleic acid was used as the model carboxylic acid for the reactions. The hydrogenation reaction was performed at room temperature. Results showed that Pd nanoparticles supported on silica were effective toward the selective hydrogenation reactions of  $\alpha$ ,  $\beta$ -unsaturated aldehydes, like cinnamaldehyde and citral which produce valuable commodity chemicals including pharmaceuticals, insect repellents, fragrances, and perfumes.

## AEI 52

## **Synthesis and characterization of polypyridinium dyes for solar cells and ruthenium catalysts based on Grubbs' first and second-generation catalyst**

**Andrew D Basner**, *adbassner@syr.edu*. Department of Chemistry, Syracuse University, Syracuse, NY 13210, United States

The redox and spectral properties of a variety of di- and triruthenium polypyridyl complexes has been studied with the goal of evaluating their potential use as dyes in dye-sensitized solar cells capable of producing photocurrent from near-IR light. A number of multi-ruthenium compounds were also prepared using the bridging ligands 2,3,5,6-tetrapyridylpyrazine (TPPZ), 2,2'-biimidazole (BIM), and 2,2'-bipyrimidine (BPM). A new, unsymmetrical polypyridyl bridging ligand, 2,3,5,6-tetrapyridylpyridine (TPPY), was prepared by performing a Stille coupling of 2,3,5,6-tetrabromopyridine with 2-(tributylstannyl)pyridine. This ligand was used to bridge two ruthenium centers, making the compound,  $[(TPY)Ru - TPPY - Ru(TPY)](PF_6)_3$ , ( $TPY = 2,2';6',2''$ -terpyridine), which has both Ru-C and Ru-N bonds to the central ring. Ligand substitution in Grubbs' first and second-generation catalyst was also performed. A number of new catalysts were made by substituting  $PBu_3$ ,  $PM_3$ , CO, and 3-bromopyridine in place of  $PCy_3$ . Ring-opening metathesis polymerization, ring-closing polymerization, and structural characterization was performed on these compounds.

### **AEI 53**

#### **Materials design by first-principles**

**Jakoah Brgoch**<sup>1,2</sup>, *jrbrgoch@mrl.ucsb.edu*, Ram Seshadri<sup>1</sup>, Gordon J Miller<sup>2</sup>. (1) Materials Research Lab, University of California, Santa Barbara, Santa Barbara, CA 93106-5121, United States (2) Department of Chemistry, Iowa State University, Ames, Iowa 50011, United States

Improvements in computational chemistry methods have provided the foundation necessary for exploring new, complex materials systems. Two approaches are generally employed when using these codes to investigate structure-composition-property relationships. The first creates a model that accurately describes the electronic structure of a known compound to further the understanding of the system. For example, my research has focused on a series of intermetallic borides that display cooperative magnetic behavior dependent on their total valence electron count. Due to the complex nature of the magnetic ordering in these metals, interpreting the magnetization data is often ambiguous. However, accurately calculating the exchange interactions at a given valence electron count, allows us to identify the magnetic ordering that best explain the data. Not only does this assist in data analysis, but it can also help us predict the magnetic ordering for unprecedented compounds.<sup>1-3</sup> The second method uses first-principles calculations as a screening tool to select compounds with a desired property without labor-intensive sample preparation. For example, oxides that have highly connected polyhedral units tend to be efficient hosts for down-conversion phosphors by shutting down non-radiative relaxation pathways. The best metric, we

believe, to compare connectivity in a structure is by approximating the Debye temperature through the elastic constants. This approach will allow us to screen oxides rapidly prior to sample preparation, a process that can save time and money as part of the search for new phosphor materials. These examples from my research experiences show how first-principles methods can be applied to various types of materials, from wide band-gap oxides to magnetic metals, and assist in the design of novel functional materials.

(1) Brgoch, J., *et al. J. Am. Chem. Soc.* **2011** , 133, 6832.

(2) Goerens, C., *et al. Inorg. Chem.* **2011** , 50, 6289.

(3) Goerens, C.; Brgoch, J., *et al. Submitted* **2013** .

#### **AEI 54**

#### **Functional supramolecular constructs of edge-binding, low-symmetry phthalocyanines, hemiporphyrazines, and the bridging ligand 1,6,7,12-tetraazaperylene**

**Thomas G. Gardner**, *dr.thomas.gardner@gmail.com*.Department of Chemistry, Gustavus Adolphus College, Saint Peter, MN 56082, United States

I am an accomplished college chemistry educator with experience teaching inorganic, organic, polymer, analytical, computational and advanced synthesis chemistry, as well as supervising synthesis research at the undergraduate and graduate level. My teaching experience also includes the special courses "Science Fiction Science", teaching the science and writing of science fiction; "Life with the Atom", about nuclear technology in our society; and "Chemistry for Engineers". My current research program as a visiting professor at Gustavus Adolphus College enlists twelve students exploring the goal of incorporating low-symmetry phthalocyanines, hemiporphyrazines and the bridging heterocyclic ligand 1,6,7,12-tetraazaperylene into functional supramolecular structures for potential electronic, catalytic, nanotechnological and biomedical applications. Pedagogical techniques for helping students develop an excitement for chemistry will be discussed.

#### **AEI 55**

#### **Transition metal ion complexes as MRI paraCEST contrast agents**

**Sarina J Dorazio**, *sdorazio@buffalo.edu*, Janet R Morrow. Department of Chemistry, University at Buffalo, Amherst, NY 14260, United States

Exogenous contrast agents are administered to patients in approximately half of all magnetic resonance imaging (MRI) clinical scans. Transition metal ion complexes are a promising addition to the repertoire of trivalent lanthanide paramagnetic chemical

exchange saturation transfer (paraCEST) contrast agents currently under development for clinical use. Following saturation of nuclear spins at a particular radio frequency, these paraCEST agents produce contrast based on exchange of labile macrocycle protons with bulk water protons. The varied response to pH in the physiological range will allow for improved diagnosis and prognosis of diseases such as cancer.

## AEI 56

### **C-H bond activation by iridium (III) complexes supported by NHC and cyclopentadienyl ligands**

**Jeremiah J Scepaniak**, *jjscapan@u.washington.edu*, **Joseph M Meredith**, **D Michael Heinekey**.*Chemistry, University of Washington, Seattle, WA 98116, United States*

Iridium (III) dimethyl complexes supported by NHC ligands and a cyclopentadienyl moiety (cyclopentadiene, tetramethylcyclopentadiene, and pentamethylcyclopentadiene) have been prepared. These complexes are utilized to generate electrophilic cationic Ir(III) complexes possessing an open site anticipated to be reactive towards C-H bonds. These complexes also serve as starting materials to form cationic Ir(III) carbonyl complexes. These carbonyl complexes exhibit CO stretching frequencies similar to those observed for the related  $[\text{Cp}^{\text{Me}_5}(\text{PMe}_3)\text{Ir}(\text{Me})(\text{CO})]^+$ . This data indicates that the NHC ligands have donor abilities similar to phosphines, and the the Ir(III) complexes are electronically poised for C-H bond activation.

## AEI 57

### **Carbon nanotube functionalization to develop electrically conductive thin films, bioorganic photodimerization of thymine to understand skin cancer, developing stereoselective synthetic methodology using zwitterionic effects and organoaluminum catalysis in tropanes to develop pharmaceuticals for neurobiological diseases such as Alzheimers and Parkinsons and educational research teaching large lectures**

**Juliet Hahn**, *JHahn@fmarion.edu*.*Department of Chemistry, Francis Marion University, Florence, SC 29502, United States*

Carbon nanotubes have been functionalized by bioorganic molecules to increase the electrical conductivity of the carbon nanotube thin films. The functionalization has been characterized by spectroscopy and electrical conductivity measurements. Electrically conducting thin films have many applications as novel materials, including solar energy and light weight electrically conductive materials with armor like properties. Photodimerization of thymine is implicated in skin cancer. A study of the simple bioorganic reaction eliminates the complications of the real biochemical system. The photodimerization is studied under different reaction conditions to simulate the effect of skin cancer lesion sensitive DNA segments. Tropanes are in a class of some 200

natural product molecules, including cocaine, which have neurobiological effects. The research is limited to developing synthetic methodology using a zwitterionic effect and organoaluminum catalysis. The synthetic methodology can be used for synthesis of a wide variety of pharmaceuticals. Educational research is limited to innovative methods of teaching large lecture sections. Many students are lost to many STEM areas by their experience in their first college science courses. The 75% of students who are not naturally scientifically gifted can be taught how to learn chemistry opening the door to many STEM areas. <http://JulietHahn.com>

## AEI 58

### **Importance of Ni(II) to *E. coli* and sulfur to *S. aureus***

**Khadine A Higgins**<sup>1</sup>, khiggin@indiana.edu, Peter T Chivers<sup>3</sup>, Michael J. Maroney<sup>2</sup>, David P Giedroc<sup>1</sup>. (1) Chemistry, Indiana University Bloomington, Bloomington, IN 47401, United States (2) Chemistry, University of Massachusetts Amherst, Amherst, MA 01003, United States (3) Chemistry and Biochemistry, Oberlin College, Oberlin, OH 44074, United States

1) *E. coli* requires nickel for three NiFe-hydrogenases that catalyze the reversible oxidation of hydrogen. High concentration of Ni(II) can be toxic to the cell and therefore has to be tightly regulated. RcnR is a 40 kDa homotetrameric transcriptional repressor that binds to DNA in the apo form and releases DNA in response to the binding Co(II) or Ni(II) resulting in the expression of the exporter RcnA and a periplasmic protein associated with export, RcnB. RcnR binds to a variety of first-row transition metals *in vitro*. Despite binding the first row transition metals, *lacZ* reporter assays determined that only the binding of Ni(II) or Co(II) results in the de-repression of *rcaA*. The results from this work suggest that there are two protein conformations that lead to DNA release one that features a M-S distance at 2.3 Å as seen for Co(II)-WT RcnR, and another with M-S distance at 2.6 Å that is typical for Ni(II) WT-RcnR. XAS and *lacZ* studies suggest that as long as either conformation is maintained when metal binds then the metal binding will result in the expression of RcnA.

2) *S. aureus* has a unique sulfur metabolism pathway as it cannot utilize sulfate as a sulfur source but can grow on thiosulfate and sulfide. The *cst* operon was recently discovered in *S. aureus* and may be involved in sulfur assimilation, sulfur trafficking and/or sulfide detoxification. This work focuses on CstA, a putative sulfur transferase that may be involved in the shuttling of sulfur as cysteine persulfides to downstream targets. NMR studies reveal that C66 and C128 are within disulfide bonding distance, consistent with a persulfide shuttling model and the TusA and RHOD domains pack against one another.

## AEI 59

### **Fundamental studies of the rearrangement and isomerization of high oxidation state Mo compounds relevant to ring-opening metathesis polymerization**

**Stefan M Kilyanek**, [smkilyanek@gmail.com](mailto:smkilyanek@gmail.com), **Richard R Schrock**.*Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, United States*

The structures of Mo alkylidene initiators for ring-opening metathesis polymerization (ROMP) have a drastic impact on the structure and properties of the polymers formed. The mechanisms of ROMP initiation and propagation have been studied for both Mo monoaryloxide pyrrolide (MAP) imido alkylidenes and Mo bis-alkoxide imido alkylidenes. The mechanism for isomerization / rearrangement of the intermediate species during propagation was found to have a dramatic effect on the polymer structure. The structure and reactivity of disubstituted alkylidenes was investigated to identify the species that are relevant to the rearrangement mechanism of Mo(IV) species that initiate ROMP.

## **AEI 60**

### **Biological interactions of gold nanoparticles (AuNPs): Understanding how engineered AuNP surface chemistry controls their biological fate and response**

**Samuel E Lohse**, [slohse@illinois.edu](mailto:slohse@illinois.edu).*Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, United States*

Gold nanoparticle (AuNP) surface chemistry (including the charge on the surface of the NP, ligand length, and the bonding between the ligand and the gold core) is a strong determinant of their ultimate biocompatibility. As a result, precisely engineering the surface chemistry of AuNPs is essential to maximize their performance in a variety of applications ranging from anti-cancer theranostics to drug delivery. Unfortunately, it is difficult to understand how AuNP surface chemistry dictates their behavior in biological systems, because exposure to biological environments changes the “pristine” surface chemistry of engineered AuNPs *via* interactions with proteins and biomacromolecules. As a result, the interaction between AuNP surface chemistry and biological systems must be examined as a series of interactions between AuNPs and different biological systems with different levels of complexity. Here, we describe a series of studies that seek to understand the connection between “engineered” AuNP surface chemistry and their subsequent interactions with biological systems on all levels of complexity: the formation of the protein corona in serum, the specific targeting of human cancer cells *in vitro*, interactions with cell membranes, extending up to their subsequent biological response in whole organisms. In particular, we examine how AuNP surface chemistry influences protein corona composition, how the photothermal heating of gold nanorods (AuNRs) changes the composition of their surrounding protein coronas, and how AuNP surface chemistry influences their biocompatibility in *S. oneidensis* and *D. magna*.

## **AEI 61**

### **Ultrafast charge separation in a cobaloxime photocatalyst supramolecular assembly**

**Anusree Mukherjee**, *mukherjee@anl.gov*, Oleksandr Kokhan, Jier Huang, Lin X Chen, David M Tiede, Karen L Mulfort. *Chemical Science and Engineering, Argonne National Laboratory, Lemont, IL 60439, United States*

Development of an inexpensive, environmentally clean alternative energy source to minimize our dependence on fossil fuel is a major challenge to society. Nature has developed photosynthetic systems to store diffuse but abundant solar energy through chemical bonds, which has inspired chemists to design compounds that can replicate the same process in abiotic compounds. Our approach toward artificial photosynthesis involves coupling photochemical modules and H<sub>2</sub>-evolving catalytic modules via supramolecular interactions. We have specifically targeted economically viable cobaloximes as the catalytic module as they have been demonstrated to be truly robust and efficient in electro- and photo-chemical pathways of hydrogen production. In this project we have investigated how fine tuning the linkage between Ru(II)polypyridyl based photosensitizers and the cobaloximes affect the functional parameters of the new supramolecular photocatalysts. The prime goal of the project is to elucidate the mechanism of light-driven hydrogen production by heteronuclear supramolecular assemblies. A variety of physical techniques will be employed to probe the ground state characteristics (electrochemistry, X-ray absorption spectroscopy, UV-visible spectroscopy) and to shed light on the nature of the transient state (transient absorption spectroscopy, time-resolved X-ray scattering). This study will give fundamental insight about the mechanism of photo-catalytic hydrogen production and will pave the way for new architectures for carrying out artificial photocatalysis.

## **AEI 62**

### **Hydrogen and methane storage in a phthalocyanine 2D covalent organic framework**

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Covalent organic frameworks (COFs) are structurally precise, crystalline materials that have attracted significant attention due to their potential applications in efficient gas adsorption (H<sub>2</sub>, N<sub>2</sub>, CO<sub>2</sub>, NH<sub>3</sub>), in catalysis, and importantly, in optoelectronic devices. A two-dimensional cobalt based phthalocyanine covalent organic framework (CoPc-BPDA COF) has been solvothermally synthesized, which exhibits high thermal stability (350°C), high porosity (S<sub>BET</sub> = 1087m<sup>2</sup>/g). The phthalocyanine core provides coordination sites for various metal ions which could potentially enhance the interaction with hydrogen for favorable hydrogen. These characteristics would make them promising candidates for gas storage.

## **AEI 63**

### **Metal clusters toward bioinorganic models and functional materials**

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Nature uses a variety of metal clusters in biological systems to perform catalysis. Nature's blueprints for functional catalysts has inspired biomimetic inorganic models or synthetic clusters in an effort to attain the activities of the biological system in a synthetic system. One such natural system is Photosystem II which uses a tetranuclear manganese cluster to achieve the efficient oxidation of water to  $O_2$ .  $Mn_4$  Cubane clusters analogues of PS II oxygen evolving system (OEC) have been isolated with 4, 5, and 6-coordinate manganese-oxo/nitrogen clusters. A second system of focus is the phosphotriesterase (PTE) enzyme, which catalyzes the hydrolysis of a wide range of phosphoesters (for paraoxon,  $k_{cat}$  2400  $s^{-1}$ ). Using a novel class of architectural metal templating ligands (spiroligomers) designed computationally and synthesized in the lab, we have been able to engineer metal complex templates for the generation of catalysts to carry out the hydrolysis of such organophosphorus compounds. Results of these model studies and future directions will be discussed.

#### **AEI 64**

#### **Rational synthetic routes to a family of tetravalent cerium amido compounds**

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Of the rare earth elements, only cerium is known to exhibit a tetravalent oxidation state in its coordination chemistry. By and large, new reports of cerium(IV) coordination compounds result from a common synthetic approach: oxidation of a related cerium(III) starting material. However, this requires extensive screening of conditions and reagents to arrive at high yielding routes to pure cerium(IV) containing products. We are working to establish rational synthetic routes in order to expand the coordination chemistry of tetravalent cerium. We have synthesized new cerium(IV) silylamido complexes by oxidation of their trivalent analogs. These complexes serve as starting materials that allow for further synthetic modifications with maintenance of the cerium(IV) oxidation state. The electrochemical and spectroscopic characterization of this new family of compounds will be discussed, as well as their reactivity and possible applications.

#### **AEI 65**

#### **Identification of novel, selective CDK5/p25 inhibitor: Structure based virtual screening, synthesis, biological evaluation and SAR studies**

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Cyclin dependent kinase 5 (CDK5) is a proline directed Ser/Thr kinase, which is expressed primarily in the central nervous system (CNS). CDK5 regulates neuronal development rather than cell division and is deregulated by its neurotoxic activator p25. As a cascade mechanism, tau protein becomes hyperphosphorylated and produces deposits of neurofibrillary tangles (NT). The deregulation of CDK5 is believed to be responsible for several neurodegenerative conditions including Alzheimer's disease, Parkinson's disease, stroke and Huntington's chorea. Because of its involvement in NT formation, the inhibition of CDK5-p25 complex has been identified as a potential therapeutic target for Alzheimer's disease. CDK5 has a high level of structural homology (~60%) with its mitotic counterpart CDK2, which has made it difficult to design selective CDK5 inhibitors. We employed structure based virtual screening of a commercial database containing 2.5 million compounds to identify a group of probable hits. Subsequently, we employed the selectivity constraints from docking scores and identified a limited number of CDK5 selective compounds. These compounds were evaluated in  $^{33}\text{P}$  labeled functional assays in order to validate the computational model. A novel, selective and non-ATP competitive CDK5-p25 inhibitor has been identified. The present study highlights the computational model, novel synthetic strategy and further SAR studies of the lead compound.

## AEI 66

### **Ionic liquid forms of active pharmaceutical ingredients in drug delivery**

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Ionic liquids (ILs, salts that melt under 100 °C) are a unique class of compounds whose chemo-physical properties can be easily varied and controlled. A wide variety of anions and cations can be used to tune the ILs for specifically targeted properties. This can be seen in the evolution of ILs from solvents (1<sup>st</sup> generation of ILs) to energetic materials (2<sup>nd</sup> generation of ILs) and further more to biological compounds (3<sup>rd</sup> generation of ILs). This presentation focuses on the application of the IL approach to active pharmaceutical ingredients (APIs) and the advantages offered for improving several properties of currently used solid APIs.

Currently, the pharmaceutical industry is facing several problems (e.g., polymorphism, low water solubility, and low bioavailability) mainly related to the solid state of the APIs. One solution to these problems is the liquefaction of solid APIs into IL-APIs which we have shown to exhibit superior properties when compared to the parent API. Combining the IL strategy with several other strategies, such as the prodrug and supported ionic liquid phase (SILP) strategies, can lead to new potential drug delivery systems. These

concepts have been supported through release studies of the parent API and of the IL-API from the solid support, respectively, into simulated body fluids.

## AEI 67

### **C-di-GMP signalling in bacteria: New opportunities for the development of antibiofilm drugs**

**Jie Zhou**, *jzhou@umd.edu. Department of Chemistry and Biochemistry, University of Maryland, College Park, College Park, MD 20742, United States*

For an organism to survive, it must sense its environment and coordinate metabolism to a changing environment. In bacteria, cyclic diguanylate (c-di-GMP) is a universal second messenger that is synthesized in the cytosol, in response to a changing bacterial environment, to regulate bacterial physiology. C-di-GMP has been shown to regulate biofilm formation as well as virulence gene expression in a variety of bacteria. Analogs of c-di-GMP have the potential to be used as chemical probes to study c-di-GMP signaling and could even become drug leads for the development of anti-biofilm compounds to treat persistent bacterial infections. Herein we reported the synthesis and biophysical studies of a series of c-di-GMP analogs. We studied both polymorphisms of these analogs using DOSY NMR and the binding to several effector proteins, such as PilZ-containing proteins, diguanylate cyclases (DGC) containing I-sites, and phosphodiesterases (PDE). We found that selective binding to different classes of c-di-GMP binding proteins could be achieved with the 2'-modified analogs and that 2'-F analog of c-di-GMP binds to the I-site of DGCs better (4 times) than the native dinucleotide, c-di-GMP. On the contrary, c-di-GMP binds to PDEs better (10 times) than 2'-F-c-di-GMP does. 2'-F-c-di-GMP potently inhibits c-di-GMP synthesis by DGCs and hence raises the potential that cell permeable analogues of 2'-F-c-di-GMP could be used to disrupt c-di-GMP signaling in bacteria.

## AEI 68

### **Application of a straightforward approach to incorporate terminal guanidines in natural product total synthesis**

**Stephen Chamberland**, *chambers@cwu.edu. Department of Chemistry, Central Washington University, Ellensburg, Washington 98926, United States*

Many natural and unnatural complex organic molecules contain terminal guanidine functional groups. Often, the affinity and specificity with which a terminal guanidine binds to the active site of a small molecule's protein target determines biological activity. In the practice of total synthesis, the basicity and nucleophilicity of the guanidine group seemingly prompts synthetic chemists to introduce this group late in their synthesis. Furthermore, the use of latent amine, such as an azide or a carbamate as guanidine progenitor can lengthen a synthetic route by several unnecessary functional group interconversions.

Because of their biological activity, intriguing structure, and accessibility by undergraduates, we have pursued the total synthesis of terminal guanidine-containing natural products such as phidianidine A and B, and clavataidine A. Frustrated by extant approaches to late-stage guanidinylation, we sought a more deliberate approach. In summary, early-stage, direct introduction of the guanidine functional group in a protected form led to streamlined total syntheses of these natural products.

## AEI 69

### Self-assembled functional nanomaterials from bis-urea macrocycles and di-block copolymers

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In my graduate research I focused on making and exploring tubular nanomaterials using *bis*-urea macrocycles. Self-assembly of *bis*-urea macrocycles give tubular crystal with nano-sized channels that can be used as molecular containers. Molecular containers alter the reactivity, stability, and chemical behavior of the reactants entrapped within them. They can absorb solid guests such as coumarin, stilbenes, acenaphthylene and styrenes from solution. These guests usually undergo non-selective photoreaction in solid-state with very low percent conversion to produce photodimers. Within our molecular container, a number of these guests showed photo-dimerizations with amazing selectivity and enhanced conversion.<sup>1,4</sup> We also investigated bipyridine containing macrocycles that have potential to form Metal Organic Framework (MOFs).<sup>2,3</sup>

In the post-doctoral study I broadened my expertise in bio-responsive soft-material self-assembly and nanolithography using block co-polymers. We designed and prepared hPB-*b*-PEO based polymeric thin film that has ability to measure the impact of cellular interactions onto this soft material. We modified the hydrophilic tail of the polymer to its –NHS ester derivative and self-assembled the polymer into bilayer films. The ester group is presented on the surface of the material and it is able to make covalent bond with the fibronectin (Fn) protein. To make a patterned Fn surface material we deliver the Fn proteins from a PDMS mold and covalently stamp it onto the NHS-conjugated film by advanced nanolithography/ transfer printing technology.<sup>5</sup>

#### References:

1. **Dawn, S.** ; Shimizu, L. S. *J. Am. Chem. Soc.* **2011**, 133, 7025-7032.
2. Tian, L.; Wang, C.; **Dawn, S.** ; Shimizu, L.S. *J. Am. Chem. Soc.* **2009** , 131, 17620-17629.
3. **Dawn, S.** ; Salpage, S.; Shimizu, L. S. *Inorg. Chem. Commun.* **2012** , 15, 88-92.

4. Dawn, S. ; Shimizu, L. S. "Selective bimolecular photo-dimerizations inside self-assembled phenylethynylene *bis*-urea macrocycles." (in preparation).

5. Dawn, S.; Bermudez, H. " Nano-patterned films from block copolymer to quantify cellular response." (in preparation).

## AEI 70

### Hydrogen bond donor organic catalysts for the discovery of new reactivity patterns

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Organocatalytic synthetic methods are attractive alternatives to transition metal catalysis. Small organic molecule catalysts not only offer complementary reactivity patterns to metals, they often benefit from being less expensive, more robust, and more environmentally friendly. Ureas, and other hydrogen bond donors (HBD), are one particularly attractive family of organic catalysts capable of effecting transformations through hydrogen bonding interactions. Despite the undeniable promise of HBD catalysis, challenges, such as high catalyst loadings and limited reactivity patterns, limit its widespread use in academia and industry. This work will present recent advances from the Mattson group in the design and utility of HBD catalysts. In particular, internal Lewis acid-assisted ureas and silanediols will be discussed with a focus on new patterns of reactivity and the synthesis of these unique HBD catalyst frameworks.

## AEI 71

### Palladium-catalyzed deprotonative cross-coupling process of allylbenzene derivatives: Overriding the Heck reaction to obtain regioselective diarylallyls

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Palladium-catalyzed cross-coupling reactions have become one of the most appreciated tools in synthetic organic chemistry. Metal catalyzed direct functionalization of  $sp^3$  C-H bonds has received much attention, and current methods to achieve direct arylation depend greatly on substrates with appropriately placed directing groups to steer reactivity. Nevertheless, considerable less success has been realized in the intermolecular arylation of weakly acidic  $sp^3$  C-H bonds in the absence of directing groups. We report herein the general, high-yielding, and scalable method for palladium-catalyzed  $sp^3$ C-H arylation of arylbenzene derivatives ( $pK_a \sim 34$ ) with aryl bromides to give the first regioselective synthesis of the  $\alpha$ -selective diarylallyl products, which cannot be synthesized by the conventional Heck reaction. Key to the success of this approach

is an in situ metalation of the substrate via C-H deprotonation under catalytic cross-coupling conditions, which is referred to as a deprotonative cross-coupling process (DCCP).

## AEI 72

### **Blocking virulence: Disruption of quorum sensing in *Pseudomonas aeruginosa***

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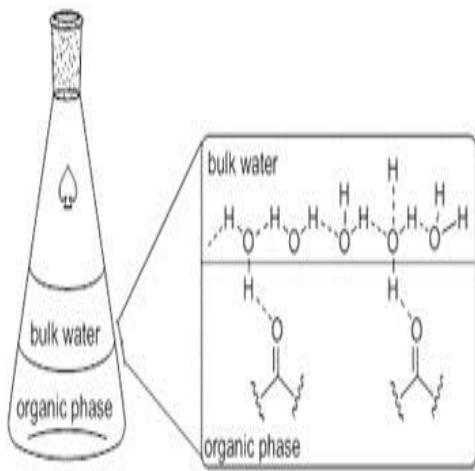
Quorum sensing is the communication process used by bacteria to control collective behaviors including bioluminescence, biofilm production, and virulence. Targeting virulence, by inhibiting quorum sensing, could constitute a new leading edge strategy to combat Gram-negative bacteria, which is of increasing importance with the rise of antibiotic resistant strains. A library of small molecules was synthesized and the compounds were investigated for their ability to block virulence in *Pseudomonas aeruginosa* by disrupting the LuxIR quorum sensing circuits, leading to the identification of new potent inhibitors.

## AEI 73

### **Water as a heterogeneous liquid catalyst: From mechanism to sustainable processes**

**Maxim O Ratnikov**, [ratnikov@scripps.edu](mailto:ratnikov@scripps.edu), **Valery V Fokin**. Department of Chemistry, The Scripps Research Institute, La Jolla, California 92037, United States

The unambiguous role of water in heterogeneous aqueous-organic catalysis is proposed. This refined mechanistic model has guided efforts towards development of metal-free functionalization of alkenes by azodicarboxylates. The kinetic data obtained by the in situ heat flow calorimetry of water catalyzed reaction of quadricyclane and diethyl azodicarboxylate is generally consistent with the Langmuir-Hinshelwood model; linear correlation of the maximum reaction rate with the stirring rate and volume of aqueous phase indicate that water acts as a heterogeneous liquid catalyst. A maximum rate decline coinciding with heterogeneous to homogeneous transition for alcohol water mixtures is consistent catalysis on water surface. Kinetic isotope effect, the relationship between the catalytic activity of aqueous-organic interface and water solutes (e.g. surfactants, ionic salts and non-ionic compounds, and polymers) as well as applications of this system for metal-free functionalization of alkenes with azodicarboxylates will be discussed.



## AEI 74

### Functionalized nanomaterials from pyridyl urea macrocycles and functionalized polyphosphazene electrolytes for lithium ion batteries

**Kinkini Roy**<sup>1,2</sup>, [kinkiniroy@polysci.umass.edu](mailto:kinkiniroy@polysci.umass.edu), Linda S Shimizu<sup>2</sup>, E Bryan Coughlin<sup>1</sup>, Khalil Amine<sup>3</sup>. (1) Department of Polymer Science & Engineering, University of Massachusetts, Amherst, MA 01002, United States (2) Department of Chemistry & Biochemistry, University of South Carolina, Columbia, SC 29208, United States (3) Chemical Sciences & Engineering Devision, Argonne National Laboratory, Argonne, IL 60439, United States

We developed *bis*-urea macrocycles that can predictably self-assemble into porous. My PhD dissertation focused on the synthesis of macrocycles that combine ureas and a second functional group (pyridine) to afford columnar assembly with functionalized pores.<sup>1</sup> Our synthesized *bis*-urea pyridyl macrocycles assembled via urea-urea hydrogen bonding and  $\pi$ - $\pi$  stacking to afford closed pack one dimensional solid nanotube with no pores. We showed that despite the lack of pores, these seemingly nonporous nanotubes can expand in presence of polar guests.<sup>2</sup> Hydrogen bonding interactions between guest alcohols and unsatisfied urea lone pairs were observed in the solid complexes and are likely the driving force for these solid-to-solid transitions. Halogen bonding can also be used to induce absorption.<sup>3</sup>

In my post-doctoral study I decided to expand my expertise on *tailoring chemical functionality to generate functional polymeric material for alternative energy*. We are interested in developing fire safe polymeric electrolytes for lithium-ion batteries. Polyphosphazenes are macromolecules that contain a backbone composed of alternating phosphorus and nitrogen atoms, and organic groups can be attached to the backbone phosphorus atoms. They have low glass transition temperatures ( $T_g$ ) and are extremely nonvolatile and less flammable. We decided to develop polymer electrolytes

by tethering oligoethylene oxide chains to phosphazene backbone. We performed two parallel lines of investigations by functionalizing cyclicphosphazene trimer as well as linear polymers. A series of cyclotriphosphazenes and polyphosphazenes bearing pure and mixed oligoethylene-oxide chains were synthesized. They have low  $T_g$  and good ionic conductivity when doped with lithium salt<sup>4</sup>.

#### Reference

- 1) Roy, K.; Shimizu, L. S. *J. Org. Chem.* **2010**, 75, 5453 (Featured Article).
- 2) Roy, K.; Shimizu, L. S. *Chem. Commun.* **2011**, 47, 277–279.
- 3) Roy, K.; Shimizu, L. S. *Chem. Mater.* **2012**, 24, 4773–4781.
- 4) Roy, K.; Zhang, Z.; Amine, K.; Coughlin, E. B. "Phosphazene Oligomers as Electrolytes for Lithium Batteries" (In preparation)

#### AEI 75

#### Silver(I)-catalyzed regioselective cyclization reactions

**Biswajit Saha**, bsaha75@gmail.com, Juzan Perez, Rachel Dipietro. Chemistry, North Central College, Naperville, IL 60565, United States

Recently, silver(Ag)(I)-salt catalyzed organic reactions have gained attention due to mild Lewis acidity, environmentally benign nature, cost effectiveness and easy availability. We have developed a general methodology for constructing mono- or di-substituted oxygen-containing heterocyclic molecules via Ag(I)-catalyzed reactions, because these type of ring structures are prevalent in biologically important natural products. Thus, we can apply our methodology for synthesizing such natural products which can be utilized in future potential drug discovery research for various diseases (e.g. cancer and malaria).

#### AEI 76

#### Silanediols as catalysts for nitroalkene activation

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Small organic molecules capable of catalyzing reactions through hydrogen bonding interactions are emerging as powerful tools in organic synthesis. Conventionally, hydrogen bond donor (HBD) catalysts have been inspired by the anion recognition abilities offered by urea, thiourea, and guanidinium functionalities. The exploration of innovative HBD scaffolds is an attractive direction in organocatalysis research to

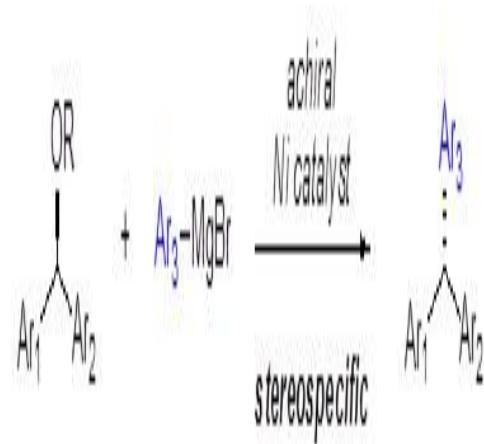
overcome barriers associated with current HBD catalysts, such as high catalyst loadings and limited reactivity patterns. Specifically, silanediols have been identified as promising HBD catalysts for the activation of nitroalkenes towards nucleophilic attack. The design behind our silanediol catalyst system, including an investigation of asymmetric catalysis with silanediols, will be presented.

**AEI 77**

### **Development of stereospecific nickel-catalyzed cross-coupling reactions of benzylic ethers**

**Buck L. H. Taylor**, *bucktaylor@ucla.edu*, **Elizabeth C. Swift**, **Michael R. Harris**, **Margaret A. Greene**, **Elizabeth R. Jarvo**. *Department of Chemistry, University of California Irvine, Irvine, CA 92697, United States*

A stereospecific cross-coupling reaction of benzylic ethers with Grignard reagents has been developed. Enantioenriched benzylic ethers, derivatives of easily synthesized chiral secondary alcohols, undergo cross-coupling with high enantiospecificity using an achiral nickel catalyst. The method has been applied to the asymmetric synthesis of biologically active diarylethanes, a common structural motif in medicinally relevant compounds. Additionally, aryl and heteroaryl Grignard reagents can be used for the synthesis of enantioenriched triarylmethanes, including an anti-breast-cancer agent. Kinetic studies will be described, providing insight into the reaction mechanism and potential improvement of this methodology.

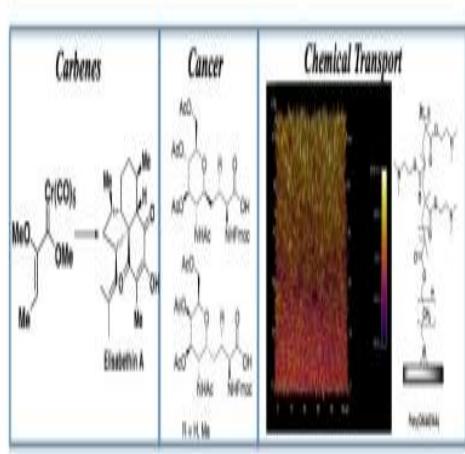


**AEI 78**

### **Carbenes, cancer, and chemical transport**

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Metal-stabilized Fischer carbenes have played an important role in organometallic chemistry and the construction of complex molecules. This poster will begin by presenting a few of these carbenes and how they can react both in annulations and in tandem cyclizations to create natural product precursors. Switching gears, RCM or CM (using a metal stabilized carbene) can lead to carbon linked glycomimetics which can act as bioconjugates toward cancer antibody formation. This poster will also present our pathway toward these C-linked mimics. Finally, towards creating an autonomous separation system we have devised a gradient grown polymer brush architecture that directs molecular transport and led to both separation of molecules and remediation of organophosphates.



**AEI 79**

### Applications of rhenium catalysts

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Environmentally benign processes require chemical transformations that feature 'green' characteristics such as catalytical, atom-economy, selective, and reusable.

Biomass is an appealing renewable and abundant carbon neutral source. Glycerol is a byproduct of biodiesel production that has been in oversupply since 1995. Environmentally-friendly and efficient conversion of glycerol (or other biomass-derived polyols such as erythritol and threitol) is desirable. In the first part, we reported on Re catalysts that can catalytically produce small and useful organics (SUO) from biomass-

derived polyols under neat conditions and reasonably mild temperatures. The main products are allylic alcohol from glycerol and 2,5-dihydrofuran from erythritol. Based on kinetic isotope effect study and control experiments, a mechanism is proposed that involves transfer hydrogenation on a bifunctional catalytic site.

Developing a clean energy supply is needed to sustain the rising global population and need for energy. Hydrogen is one of the most promising and green fuels. A series of Rh, Ir homogeneous catalysts have been used for the dehydrogenation of alcohols. Modification of the ligand has provided some insight and control on reactivity. However, very limited studies on Re-catalyzed dehydrogenation of alcohols are available. We will present a robust and fully recyclable Re catalyst that produces directly dihydrogen and ketone from alcohol under neat conditions.

## **AEI 80**

### **Laser spectroscopy and imaging techniques studying chemicals and dynamics of chemical reaction in gas and condensed phases**

**Ming-Wei Chen<sup>1</sup>**, *mingchen@illinois.edu*, **I-Chia Chen<sup>2</sup>**, **Jinjun Liu<sup>3</sup>**, **Terry A. Miller<sup>4</sup>**, **Dana D. Dlott<sup>1</sup>**. (1) Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801, United States (2) Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan Republic of China (3) Department of Chemistry, University of Louisville, Louisville, KY 40292, United States (4) Department of Chemistry, The Ohio State University, Columbus, OH 43210, United States

Chemicals emitted into the environment from both biogenic and anthropogenic sources are recognized to contribute to photochemical air pollution, acid rain, ozone depletion in the stratosphere, and material corrosion. These effects are followed by a complex array of chemical and physical transformations, and harmful to the human health and environment. To understand the mechanism of these photochemical processes and characterize the roles of the molecules in these reactions are essential to the fundamental science interests and to the applications such as the environmental and material protections.

In my graduate researches, different laser spectroscopy techniques were developed depending on the needs of experiments for molecules of interest, such as laser induced fluorescence, stimulated emission pumping, cavity ringdown. With adequate laser spectroscopy techniques used, the pollutant chemicals can be studied in laboratory. Some of my research accomplishments are: the formyl radical formation at near dissociation threshold of glyoxal photoexcitation, spectroscopic characterization of methoxy radical at electronic ground and first excited states including the spin-orbit components, and vibrationless photoexcitation induced dynamics of  $\beta$ -hydroxyethylperoxy were studied and published.

Currently, my postdoctoral research focus is combining my experience in laser spectroscopy and optics to develop a thermal/IR imaging microscope apparatus to

study the hotspot generation in solid energetic materials. Hot spot generation in energetic material is an important process to initiate the exothermic chemical reaction, but less knowledge is known about the mechanism with loading weak energies. We utilize a far-IR laser to initiate the hot spot generation in the 1,3,5-trinitroperhydro-1,3,5-triazine (RDX) crystals, and have successfully observed the hot spot growing in crystals.

Besides the above accomplishments, there are still ongoing projects and further results forthcoming. Moreover, integrating all my knowledge in physics, chemistry and experimental developments for researches, these experiences can also be used to investigate fields for the scientific challenges.

## AEI 81

### **Materials chemistry by pulse visible and IR lasers: CPCD (confined plume chemical deposition) and LCVD (laser chemical vapor deposition)**

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The poster will discuss our results on materials chemistry by two laser chemical deposition methods - CPCD (Confined Plume Chemical Deposition) and LCVD (Laser Chemical Vapor Deposition). Comparison will be made between the two approaches including advantages and disadvantages of each of the two methods. The lasers used include Mid IR tunable picosecond Free Electron Laser, 800 nm Ti:sapphire femtosecond laser, 532 nm SHG of Nd:YAG nanosecond laser, 510/578 nm nanosecond CuBr vapor laser and 2.94  $\mu$ m Er:YAG microsecond laser. The deposited materials include polycrystalline ReB<sub>2</sub>, RuB<sub>2</sub>, WB<sub>4</sub>, B<sub>4</sub>C, and Ge on variety of inorganic (Si, Glass, NaCl and Cu), polymer (HDPE, UHMWPE and PTFE) biological (bone and onion) substrates. To the best of our knowledge's this is the only way high temperature crystalline borides can be directly deposited on polymer and biological substrates without visibly destroying underlying surface. Possible mechanism behind CPCD will be discussed. Proposal for building of new kind of pulse laser phase diagram for any material which include not only average power of the laser (or average energy density) but also wavelength, energy per pulse, pulse duration and repetition rate will be considered. Future directions of research for CPCD and LCVD will be presented.

## AEI 82

### **EPR study of nitroxide-labeled brush polymers**

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Bottle-brush polymers are highly branched polymers, which possess a high density of polymer side chains uniformly grafted to the backbone of a linear polymer. Functional groups can be attached to different domains of the bottle-brush polymers for potential applications that range from nanomedicine to molecular electronics. We are interested in how the locations that the functional groups are placed in bottle-brush polymers affect their reactivities and interactions with surrounding environment. The results of the study will impact further development of bottle-brush materials as nanoscaffolds for biological applications.

We synthesized bottle-brush polymers with nitroxide probes covalently attached to variable locations of the polymers: backbone middle, backbone end and side-chain end etc. Electron paramagnetic resonance (EPR) spectroscopy was used to study spin dynamics of the nitroxide probes. Parameters extracted from EPR spectra clearly indicate that the spin mobility is greatly influenced by the density of near brushes of the polymer. The results are further confirmed by a redox reaction that shows different reactivities at different locations that the probe was attached.

## **AEI 83**

### **Guiding the development of anion exchange membrane fuel cells with molecular dynamics simulations**

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The escalating climate crisis and limited supply of fossil fuels have made it imperative that alternative energy technologies be developed. In particular, by replacing combustion engines and powering personal electronic devices, anion exchange membrane (AEM) fuel cells could be an important component of a long-term, clean energy strategy. Molecular dynamics simulations can provide important atomic resolution details about the structure and dynamics of these systems to aid in developing, characterizing, and optimizing these materials. The work presented will feature two major components: the development of methodologies to increase the efficiency and accuracy of simulations of these systems, and the application of computational methods to systems related to the development of fuel cell membranes. AEMs enable the transport of hydroxide from the cathode to the anode, which involves bond breaking and forming events. Classical interaction models are not equipped to deal with reactions, so it was necessary to develop a reactive model of hydroxide. Also an approach that dramatically increases the efficiency of free energy calculations by

optimizing the protocol used to connect two states of interest will be presented. These methods are paired with molecular dynamics simulations to describe the effects of concentration and counterions on anion transport in aqueous solutions of hydroxide salts and alkylammonium salts. Last, the solvation structure and dynamics of hydroxide are characterized in AEMs with the aim of connecting membrane composition and characteristics to the desired hydroxide transport properties. The results from these atomistic simulations will be coupled with macroscopic observables from experiment to characterize the performance of AEMs and suggest possible improvements to advance fuel cell technologies.

## AEI 84

### Spectroscopic analysis of a natural product: Anethole

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Anethole [*E*-1-methoxy-4-(1-propenyl)benzene] is a natural product molecule that is commonly recognized as the flavor component of anise, fennel, and licorice. This molecule is insoluble in water, but highly soluble in ethanol, leading to spontaneous emulsification in ethanol/water solutions (Ouzo effect). The molecular level explanation of this behavior is derived from the relative strength of intermolecular forces. My group is currently studying the unique inter- and intra- molecular forces observed in anethole.

Here, we report the jet-cooled, laser-induced fluorescence and single vibronic level fluorescence spectra of anethole. Analysis of the spectra confirms the existence of two rotational isomers that differ by the relative orientation of the methoxy and propenyl groups. The observed vibronic activity of anethole is similar to that of styrene, indicating planar symmetry of both rotamers of anethole. Interestingly, spectral signatures of water clusters with anethole can be observed in samples of 'pure' anethole. Spectral assignments in this study are assisted by density functional theory and *ab initio* calculations.

## AEI 85

### Measuring electrostatic fields at protein interfaces using vibrational Stark effect spectroscopy

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Local protein electrostatic fields play an important role in protein functions including folding, chemical reactivity, enzyme kinetics, and protein-protein interactions making measurement of these fields in a protein of interest a longstanding goal of the biophysical community. Vibrational Stark effect (VSE) spectroscopy is used to measure electrostatic fields at protein-protein and protein-solvent interfaces; the absorption

energy of a probe in a reference and perturbed system is measured and the difference is correlated to a change in electrostatic field caused by the perturbation.

Protein-water interactions impact protein structure and function as proteins typically sequester hydrophobic amino acid residues and expose hydrophilic or charged residues at the surface. Nine interfacial locations were chosen on a model protein, RalGDS, placing each probe in locations where the high dielectric constant of the solvent changes dramatically to low dielectric environment of the protein. In this study, we change the solvent dielectric constant, through the addition of known amounts of glycerol, resulting in a change in absorption energy for each probe corresponding to the angle the probe makes with the protein surface and its solvent accessible surface area.

The formation of a proper protein-protein interface controls binding discrimination. Ras and Rap have the ability to bind to the same downstream effector proteins with dissimilar dissociation constants and free energies in spite of a high degree of structural similarity. A single-charge reversion mutation at amino acid 31 has been shown to reverse binding discrimination to downstream effector proteins such as RalGDS. For both Ras and Rap three mutant variants were constructed: a double reverse mutation at positions 30 and 31, along with the two corresponding single mutations. Each mutant was bound to RalGDS, containing a VSE probe, and the absorption energy of each RalGDS/mutant pair was compared to the RalGDS/wildtype pair, resulting in three distinct trends.

## AEI 86

### **Self-assembled monolayers: A simple foundation for fundamental and applied studies**

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Self-assembly refers to the organization of molecules into two- and three-dimensional structures based on non-bonding interactions. Cell membranes are an example of this phenomenon in nature, as phospholipids are driven to form structures through hydrophilic and hydrophobic interactions between phospholipids and the aqueous environment. Similarly, molecule-molecule and molecule-surface interactions order molecular species on surfaces to form films. Self-assembled monolayers (SAMs) are easily prepared and can be easily modified, making them ideal for creating interesting and technologically useful surface architectures for use in a variety of fields as diverse as molecular electronics and bio-related applications.

My research has focused on fundamental and applied research on these self-assembling systems. As a graduate student, I used scanning tunneling microscopy (STM) to characterize bi-component, SAMs formed through various deposition procedures to better understand the kinetic and thermodynamic influences on the ordering of these systems. My research as a postdoctoral fellow has focused on the

application of these films towards developing biological surfaces that will improve protein-substrate interactions. Proteins are able to express catalytic and sensing functions that current technologies are unable to reproduce; proteins tend to lose function on inorganic surfaces due to unfolding, aggregation, and overall loss of structure that occurs when a soft, solution-phase material is placed in the harsh structural and electrostatic environment that occurs on and near non-biological surfaces. In our group, we have developed a surface that is composed of peptides that can be tailored for specific and directed protein attachment. The peptide-functionalized surface is created on an alkanethiol scaffold, attached via a Huisgen cycloaddition reaction that tethers the peptide to reactive terminal groups on the monolayer. We have incorporated a number of surface analysis techniques — vibrational spectroscopy, circular dichroism spectroscopy, x-ray photoelectron spectroscopy, and STM — to characterize chemical composition, as well as peptide orientation, conformation, and spatial distribution.

## **AEI 87**

### **Beyond basic molecular dynamics: New tools for the study of molecules in motion**

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Since the 1930s, theorists have studied chemical processes using molecular dynamics. However, many interesting problems cannot be studied from these straightforward classical nuclear trajectories. Classical mechanics has no concept of the quantum electronic states needed to describe many energy transfer problems, nor does it have the ability to capture quantum effects in the motion of light nuclei. In other cases, such as protein folding and many other biological processes, classical dynamics might be theoretically sufficient, but multiple intermediates and the rareness of each transition makes study by naive molecular dynamics intractable, even with modern supercomputers.

My research has developed new techniques which extend basic classical molecular dynamics to rectify these problems. I have developed tools to perform classical simulations of nonequilibrium quantum transport, to study the importance of quantum coherence effects in molecular motion, and to efficiently calculate the rates involved in networks of rare events. These fundamental methodological techniques are relevant to a wide range of applications, including my own interests in molecular electronics, photosynthesis, and molecular recognition in biological systems.

## **AEI 88**

### **Energy transfer in molecular photovoltaics, carbon nanotubes, and nanowires: A first-principles perspective**

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The ability to tune electronic properties in molecular photovoltaics and nanomaterials holds great promise for incorporating these materials in next-generation transistors, circuits, and nanoscale devices. In particular, the use of predictive first-principles calculations plays a vital role in rationally guiding experimental efforts to optimize energy harvesting in nanoscale and mesoscale materials. In this presentation, I highlight my recent work in using various quantum-mechanical approaches for understanding and predicting the electronic properties in light-harvesting molecules, functionalized carbon nanotubes, and heterostructure nanowires. First, I demonstrate that both the optical properties and excitation energies in photovoltaic molecules can be accurately predicted by constructing new exchange-correlation functionals for time-dependent density functional theory (DFT). Next, the use of large-scale DFT calculations is presented to understand optical detection mechanisms in chromophore-functionalized carbon nanotubes. Through joint experimental-theoretical studies, I show that a single-walled carbon nanotube functionalized with light-sensitive chromophores can function as a sensitive nanoscale color detector, where the chromophores serve as photoabsorbers and the nanotube operates as the electronic read-out. Finally, a new theoretical approach is presented to understand electron localization effects in heterostructure nanowires. At nanoscale dimensions, the formation of mobile electron gases in AlGaN/GaN core-shell nanowires can lead to degenerate quasi-one-dimensional electron localization, in striking contrast to what would be expected from analogy with bulk heterojunctions. The reduction in dimensionality produced by confining electrons in these nanoscale structures results in a dramatic change in their electronic structure, leading to novel properties such as ballistic transport and conductance quantization.

## **AEI 89**

### **Dynamics and timing: A tale of two studies**

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Multi-scale material simulations comprise the bridge between the microscopic length and time scale, and the macroscopic world. The first part will show how real-time trajectory calculations have provided for the first time a detailed dynamical picture of organic reactions involving cycloadditions [1-5]. For example, in 1,3-dipolar cycloadditions, the previously reported linear correlation between activation barriers and the energy required to distort the reactants to their transition-state geometries is now understandable in terms of the requirement for vibrational excitation [2,3]. In the case of carbene cycloadditions, we explored the range of geometries sampled in productive trajectories, as well as the timing of bond formation [4].

The second part will focus on large material simulations such as TiO<sub>2</sub> surface and polyurea aerogels. An analytic potential energy function for dimethyl methylphosphonate (DMMP) interacting with TiO<sub>2</sub> surface were developed, based on accurate cluster models[6]. Another project focuses on the assembly of polyurea aerogels. Atomistic simulations and micropores analysis helped determining the internal structure of nanoparticles[7,8].

- [1] D. H. Ess, S. E. Wheeler, R. G. Iafe, L. Xu, N. Celebi-Olcum and K. N. Houk, *Angew. Chem. Int. Ed.* 2008, 47, 7592
- [2] L. Xu, C. E. Doubleday, K. N. Houk, *Angew. Chem. Int. Ed.* 2009, 48, 2746 (highlighted by **Nature Chemistry**)
- [3] L. Xu, C. E. Doubleday, K. N. Houk, *J. Am. Chem. Soc.* 2010, 132, 3029.
- [4] L. Xu, C. E. Doubleday, K. N. Houk, *J. Am. Chem. Soc.* 2011, 133, 17848.
- [5] K. Black, P. Liu, L. Xu, C. E. Doubleday, K. N. Houk, *Proc. Natl. Acad. Sci.*, 2012, 109, 12860 (featured in **Computational Chemistry Highlights**, ScienceDaily)
- [6] L. Xu, L. Yang, W. A. DeJong, W. L. Hase, N. Govind, L. Hans, D. Tunega, *J. Phys. Chem. C*, under revision
- [7] L. Xu, C. Sotiriou-Leventis, and N. Leventis, manuscript in preparation
- [8] L. Xu, C. Sotiriou-Leventis, and N. Leventis, manuscript in preparation

## AEI 90

### Post-processing electrospun chitosan fibers for filtration applications

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Electrospinning is a simple, inexpensive, scalable and flexible method of producing fiber mats. Electrostatic forces are employed to fabricate mats, which intrinsically have larger surface area-to-volume ratio and smaller pores than commercial fibers. The prospects for market growth of fibrous mats are in areas of biomedical engineering, food processing, bacterial control and microfilters for treatment of waste or contaminated water.

Effective microfiltration depends on material structure and properties and thus, the advent of newer applications necessitates the need to find ways to improve mat reactivity, integrity and porosity. Chitosan is environmentally friendly, biocompatible, renewable and biodegradable polymer with excellent heavy-metal ion chelating abilities. Chitosan possesses functional groups increasing its reactivity and specificity, and can

also be electrospun. Combining the porous structure of the randomly oriented, electrospun chitosan fibers and improved chemical reactivity by functional group modification promises reactive and porous microfiltration membranes.

We have chemically and physically post-processed chitosan for improved chemical and mechanical stability. Chemical crosslinking was performed using stimulus responsive crosslinkers such as genipin, hexamethylene-1,6-diaminocarboxysulfonate(HDACS), epichlorohydrin, glycerophosphate, tripolyphosphate and tannic acid. Mat morphologies and chemistries were investigated under FESEM, EDS, FTIR and NMR. Mechanical properties, chemical stability, heavy metal chelating ability of the mats were determined using an Instron tensile tester, UV-Vis and ultrafiltration flow cell/EDS, respectively.

The major impacts include: (1)full chemical and tensile property analysis of the aforementioned crosslinkers with chitosan fibers; (2) introduction of four methods of processing crosslinked electrospun chitosan; (3)evaluation of the porosity and integrity of crosslinked and electrospun chitosan; (4)hexavalent chromium ion filtration profile using HDACS-crosslinked chitosan; and (5)applying knowledge of the system to design composite fibers for filtration applications. Future directions are aimed at optimizing and tailoring the structure and properties of nanofibers and their composites for tissue scaffolds engineering, controlled drug or particle delivery, active food packaging and filtration/separation applications.

## AEI 91

### **Polymer-based soft materials: Coacervate assemblies, carbon nanotube nanocomposites**

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The intelligent use of processes such as self-assembly, combined with the ability to manipulate the chemical structure of polymers, can lead to a wide array of materials. Such functional materials could be a solution to many of the challenges that the modern world faces, including improved biomedical devices and strategies for renewable energy. Here, we present two types of polymer-based soft materials that combine these two elements: polyelectrolyte self-assembly and nanocomposite materials. In the first case (work in M. Tirrell's lab), complex coacervation (i.e. a liquid-liquid phase separation phenomenon) has been utilized as a platform for soft material design. Using polypeptides as a model system we have studied many aspects of complex coacervation. We explored the thermodynamics of coacervate formation, identified how external parameters affect complexation, and studied the rheological and interfacial properties. More complex molecular design has been utilized wherein polyelectrolyte

domains are connected to neutral polymer blocks. These neutral domains stabilize microphase separation of the coacervate phase. For example, mixing of a polypeptide block-copolymer with an oppositely charged polypeptide homopolymer resulted in the formation of nanometer-sized micelles or hydrogels with coacervate core domains. The second case (work in N. Hadjichristidis' and J. Mays' labs) includes the development of a carbon nanotube (CNT) polymer functionalization strategy that helps circumvent CNTs' inherent insolubility, and considerably widens the scope of nanocomposite materials that can be produced. The strategy involved covalent attachment of substituted benzocyclobutenes to CNTs using a Diels-Alder [4 + 2] cycloaddition reaction. With a judicious choice of substitution, initiators for most popular polymerization techniques were attached onto the CNT surface. Complete control over grafting percentage of initiator and surface-initiated polymerizations allowed synthesis of nanocomposite materials with desired compositions, which is essential for any application. The resulting nanocomposite materials exhibited improved mechanical and thermal properties when compared to pure polymers.

## AEI 92

### Property control of single-walled carbon nanotubes through synthesis

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Single-walled carbon nanotubes (SWCNTs) have enormous potential for application in electronic applications such as field effect transistors, but the mixture of metallic and semiconducting nanotubes in bulk limits the reproducible production of these devices.

The electronic property (such as bandgap) of pristine SWCNTs is based on the size and chirality. Our main objective is to control the properties, including sizes, chiralities and electronic properties of SWCNTs through synthesis and to meet the need for certain electronic applications.

The size and chirality control of SWCNTs can be fulfilled by choosing appropriate catalysts and carbon sources. The bandgap changing with SWCNT diameter is not as sensitive in the large-diameter range ( $>1.5\text{nm}$ ) as in small-diameter range ( $<1\text{nm}$ ), which makes large-diameter tubes more suitable for some electronic device design. We present a method of synthesizing large-diameter SWCNTs ( $>3\text{nm}$ ) with small bandgap ( $<0.5\text{ eV}$ ) through Co-MCM41 catalysts.

The most accurate control of size and chirality of SWCNTs is from SWCNT-templated growth. The SWCNTs were shortened using liquid-phase oxidative/ mechanical cutting, which gave a tube length distribution of 50-200 nm. The shortened SWCNTs were then impregnated with cobalt catalysts and uniformly deposited onto fumed silica to form

regrowth seeds. The regrowth seeds were pretreated by hydrogen followed by ethanol pyrolysis at different temperature initiating regrowth. After regrowth, the highest yield increased by 4 times.

Though the bandgap of pristine SWCNTs is based on the size and chirality, it can be tuned (more metallic or more semiconducting) by doping carbon nanotubes with nitrogen or boron. Herein we are also presenting a method of in-situ doping of SWCNTs through Ethanol Pyrolysis.

Transmission Electron Spectroscopy, Temperature-programmed Reduction, conductivity measurement, Raman spectroscopy, photoluminescence excitation and X-ray adsorption spectroscopy will be used as the characteristic methods.

## **AEI 93**

### **Biomodulatory materials**

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As the field of biomedical engineering moves forward and tackles grand challenges like targeted intracellular delivery and organ regeneration, there exists a need for novel, multi-dimensional strategies to be developed. Current biomedical engineering solutions comprised of one biomaterial with basic structure performing a single task are suboptimal for carrying out high-order biologically-relevant functions. Instead new systems must be composed of multiple biomaterials with complex molecular-, nano-, and micro-architecture capable of performing a variety of tasks with desirable spatiotemporal control. This increase in complexity means that next generation technologies require research-based approaches from a variety of scientific fields integrated together in order to be successful.

Due to my diverse research background, I am uniquely qualified to design and develop novel solutions for complex biomedical engineering. From investigating the effect polymer chemistry has on immune cell activation and vaccine delivery as a graduate student to engineering biomaterials chemistry to facilitate musculoskeletal regeneration and induce desirable immune responses as a postdoctoral fellow, my research to date has focused on how materials properties can greatly alter their biological functionality. These previous experiences have provided me with a foundation to develop new strategies involving the design and utilization of biomodulatory materials, systems intrinsically capable of inducing desirable biological changes. During the poster session I will highlight examples of my previous research experience in this field as well as outline my future plans for building a distinguished, independent research program at the interface of chemistry, engineering, materials science, and biology. In specific, I will discuss how biomaterials chemistry and architecture can be tailored to improve immunoengineering and tissue engineering systems and how combinatorial design and evaluation techniques can be utilized to expedite research progress in these fields.

## AEI 94

### Manipulating light with polymeric materials

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The technologies that shape our future will increasingly involve the manipulation and utilization of visible light in areas such as computing, telecommunications, energy production, and biological imaging. Therefore, developing materials and systems to control and harness this energy is not simply a challenging avenue of fundamental scientific pursuit, but an opportunity to affect real social change with a large positive human impact. Organic materials are well suited to this task as the energies involved in many of their electronic transitions correspond well to the energy range spanned by the visible spectrum. In addition, they allow for many tailored properties on the molecular level such as optical bandgaps, emission properties, stimuli response, and electrical transport. Polymers are ubiquitous in a wide array of applications due to their ease of processing, robust mechanical properties, and tailored chemical functionality. Synergistic coupling of molecular-based properties with supramolecular assembly strategies and creative processing techniques allows for creation of hierarchical materials with a greatly expanded range of properties and functionality. In light of these concepts, research covering macromolecular systems capable of upconversion of visible light, mechanochromic stimuli response, data storage, photonics, and laser emission are presented.

## AEI 95

### Spatial and temporal regulation of a controlled radical polymerization by light

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Controlled radical polymerization processes have emerged as one of the most powerful synthetic strategies for the preparation of functional materials. The ability to regulate these processes with an external stimulus would dramatically increase their utility and facilitate an even greater range of applications. This poster will detail the development and applications of a practical radical polymerization process that affords both spatial and temporal control over the chain growth process through mediation by light. Insight

into catalyst structure activity relationships for this reaction, as well as applications that take advantage of the spatial and temporal control allowed by this system will be detailed.

## AEI 96

### Polymeric microcapsules with programmable active release

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We present a new type of microcapsule programmed with a tunable active release mechanism. The capsules are triggered by a plasticizing stimulus which induces a phase change transition of the polymeric membrane from a solid to a fluidized form; thereafter, the cargo is actively driven out of the capsule through a defect at the capsule wall with controllable release kinetics. Tuning the degree of membrane fluidity by tailoring the amount of plasticizing stimulus present allows us to obtain temporal variation of the release kinetics from a sub-second abrupt burst release to a slow sustained release of encapsulant over many minutes. Moreover, we demonstrate tuning of the collective capsule triggering response by adjusting stimulus content, polymer molecular weight and capsule membrane thickness. For this model system, we use a microfluidic approach to fabricate polystyrene capsules triggered by a toluene stimulus. However, this active release approach is general and is applicable to diverse polymeric capsule systems; this versatility is demonstrated by extension of our trigger-release scheme to capsules fabricated from a rubber-like block copolymer. The utility of our technique further enhances the potential of these active-release capsules for practical application.

## AEI 97

### Free radical oxidation of 7-dehydrocholesterol and its role in human diseases

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Lipid peroxidation plays important roles in the pathophysiology of common human diseases such as atherosclerosis, diabetes, Alzheimer's, Parkinson's disease, etc. In our study on free radical-mediated lipid peroxidation (autoxidation) reactions, 7-dehydrocholesterol (7-DHC), the immediate biosynthetic precursor to cholesterol, was found to be the most reactive lipid molecule known to date toward free radical oxidation. It is oxidized ca. 200 times faster than is cholesterol, and more than 10 times faster than

arachidonic acid. Autoxidation of 7-DHC in solution leads to over a dozen oxidation products (i.e., oxysterols) *via* a complex reaction mechanism, and these oxysterols exert a variety of biological activities, including cytotoxicity and induction of gene expression changes in cells.

7-DHC is accumulated in individuals affected with Smith-Lemli-Opitz syndrome (SLOS), a metabolic disorder that is caused by mutations in the gene encoding 7-DHC reductase. A number of novel 7-DHC-derived oxysterols were recently identified in cell and animal models for SLOS. Metabolic studies suggested that some of these oxysterols were originated from free radical oxidation, while others were formed *via* enzymatic oxidation catalyzed by cytochrome P450. Significantly, antioxidant supplementation was found to suppress the formation of the non-enzymatically-formed oxysterols in fibroblasts from SLOS patients. ***My current research*** focus on establishing metabolic signatures of SLOS cells and tissues using advanced mass spectrometry, elucidating the biological actions of the endogenously formed 7-DHC-derived oxysterols, and developing therapeutic approaches through the inhibition of the formation of these oxysterols in animal models of SLOS. The outcome of these lines of research is expected to shed light on other human diseases that are associated with elevated levels of 7-DHC, such as cerebrotendinous xanthomatosis, breast cancer, skin diseases, etc.