

*Poster #	Name	AGFD	ANYL	BIOL	BIOT	CARB	CATL	CHAS	CHED	COLL	COMP	ENVR	FUEL	GEOC	INOR	MEDI	ORGN	PHYS	PMSE	POLY	TOXI
1	N. Xiang	•									•										
2	J. Ashby		•	•																	
3	J. Dong		•	•											•			•			
4	D. Robinson		•				•			•						•		•			
5	O. Sathoud		•																		
6	K.H. Tran-Ba		•	•													•			•	
7	Y. Yang		•		•													•	•		
8	S. Martin			•													•	•	•		
9	J. Meisel			•													•	•	•		
10	S. Smith			•												•					
11	G. Wiedman		•	•	•												•				
12	A. Tuley			•																	
13	H. Alzubaidi		•					•				•			•						
14	M. Wilburn							•					•								
15	X. Zhang						•	•					•		•						
16	S. Zhuang							•													
17	J. Xian									•											
18	A. De Silva Indrasekara		•							•					•			•			
19	Y. Lyu		•	•																	
20	K. Phillips										•										
21	P.K. Routh		•													•					
22	S. Sharma										•										
23	T. Wijethunga									•											
24	T.E. Balias										•						•	•			
25	D. Ranasinghe										•								•		
26	N Sizochenko										•						•				
27	L.Z. Tan										•							•	•		
28	A.C Davis		•						•		•	•					•	•			
29	A. Aneksampant				•							•			•						
30	C. Davis	•									•	•								•	
31	N. Dissanayake		•								•				•					•	
32	A. Kennicutt											•									
33	C. McDonough		•									•								•	
34	M. Qin						•					•									
35	M. Shreve												•								
36	H. Wei			•									•								
37	J. Werber												•	•							
38	E. Khlebnikova											•		•							
39	J. Caranto				•											•					
40	M. Carlson																•				
41	J. Chen									•						•				•	
42	R. Comito									•						•	•		•		
43	H. Djieutedieu		•											•		•			•		
44	S. Dorazio															•		•			
45	G. Elpitiya		•													•					

*Poster #	Name	AGFD	ANYL	BIOL	BIOT	CARB	CATL	CHAS	CHED	COLL	COMP	ENVR	FUEL	GEOC	INOR	MEDI	ORGN	PHYS	PMSE	POLY	TOXI
46	E. Hernandez-Pagan																				
47	M. Jurow									●			●		●		●				
48	A. Nano													●	●	●	●				
49	S. Patwardhan								●				●					●			
50	J. Pratt									●						●					
51	J. Scepaniak													●	●	●					
52	Y. Shen									●					●						
53	P. Smith							●					●		●						
54	E.C. Tse	●	●					●	●				●		●			●			
55	W. Zhou													●	●			●			
56	S. Munoz													●							
57	J. Lee									●					●						
58	K. Teske														●						
59	R. Fuanta					●									●						
60	A. Aeby																	●			
61	M. Daub																	●			
62	M. Doud					●										●	●				
63	J. Foy																●	●			
64	S. Jianrattanasawat														●		●				
65	J. Jordan															●	●	●			
66	H. Lin																●				
67	O.M. Ogbu												●				●				
68	T. Perera																●				
69	R. Quach																●				
70	J. Schneider															●	●	●		●	
71	S. Varjosaari															●					
72	J.M. Artes Vivancos	●	●															●			
73	M. Backlund																	●			
74	K. Brorsen													●				●			
75	S. Edington			●														●			
76	B. Jones		●															●			
77	Z. Lin													●		●			●		
78	J.P. Palafox-Hernandez									●	●							●			
79	S. Perry		●															●			
80	C. Rich									●								●			
81	R. Richard													●				●			
82	H. Acar					●										●			●		
83	P. Cao																●	●	●		
84	M. Ecker																	●	●	●	
85	M. Mazzotta															●		●	●	●	
86	D. Mozhdehi					●											●	●	●	●	
87	C. Rosu													●				●	●	●	
88	M. Sadati													●					●		
89	A. Tibabuzo							●													
90	J. Vieregg					●	●												●		
91	W. Xu																		●	●	

2017 AEI Biosketches

1. Ning Xiang, Dept. of Agricultural and Biological Engineering, Purdue University, 500 Central Dr., West Lafayette, IN 47906. xiangn@purdue.edu, 765-337-3486; Hunan Agricultural University (B.S., 2011); Wageningen University (M.S., 2013), Dr. Harry Gruppen and Dr. Peter Wierenga, The effect of globular protein conformation and solution conditions on microbial transglutaminase induced cross-linking; Purdue University (Ph.D., 2017), Dr. Ganesan Narsimhan, Investigation of interaction between peptides and lipid membranes. College of Engineering Outstanding Graduate Student Research Award, Purdue University (2017).
<https://www.linkedin.com/in/ning-xiang-376b005a/>

I am interested in food colloids, food nanotechnology, novel encapsulation and delivery systems and propose to (i) characterize interfacial and colloidal phenomena using both experimental and computational methods, and (ii) develop structural design approaches to improve emulsion stability and performance. I have mentored five undergraduate and graduate students and worked as a graduate teaching assistant for three classes. I seek a tenure-track faculty position at a four-year college or university. I am also open to a postdoctoral position in the above research areas.

AGFD, COLL, COMP

Abstract Title: *Identification of antimicrobial peptide from soy protein*

2. Jonathan Ashby, Dept. of Chemistry, Mount Holyoke College, 50 College St., South Hadley, MA 01075. jashby@mtholyoke.edu; Trinity College, Hartford, CT (B.S., 2009); University of California, Riverside (Ph.D., Anyl Chem, 2014), Dr. Wenwan Zhong, Development of high-throughput methods for probing biomacromolecular interactions; NSF Graduate Research Fellow at University of California, Riverside (2011–2014); Postdoctoral Fellow at UC, Davis (2014–2016), Dr. Sheila David, Usage of non-cleavable transition state analogs of DNA lesions for affinity purification-mass spectrometry of DNA repair enzymes from cellular lysate; NIH T32 Postdoctoral Fellowship in Oncogenic Signaling and Chromosome Biology at UC, Davis (2014–2015); Ford Foundation Postdoctoral Fellowship at UC Davis (2015–2016); Consortium for Faculty Diversity Postdoctoral Fellowship, Mount Holyoke College (2016–present). UNCF/Merck Undergraduate Science Research Scholarship, Trinity College (2008–2009).

<https://sites.google.com/mtholyoke.edu/ashbylab>

My research interests lie in developing high-throughput, low-cost methods to act as prescreens to more expensive, specialized analyses. One method uses amino acid–specific tags to probe protein structural changes, as well as investigating protein–protein interfaces. I am also interested in identifying aptamers that undergo conformational change upon binding to small molecules, to be applied to rapid spectroscopic screens. These methods are being designed for ease of use, making them highly suitable for undergraduate research at a primarily undergraduate institution. I have developed several experiments for quantitative and instrumental analysis courses, where the focus is on comparison of different methods for the analysis of a class of compound. I am interested in teaching and doing research at a primarily undergraduate institution, particularly small liberal arts colleges.

ANYL, BIOL

Abstract Title: [*Fluorescamine-based screening of protein-protein interfaces*](#)

3. Juyao Dong, Dept. of Chemical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA 02139. juyao@mit.edu; Nanjing University, China (B.S., great honor, 2009); UCLA (M.S., 2012; Ph.D., dissertation award, 2014), Dr. Jeffrey I. Zink, Physical properties of mesoporous silica nanoparticles for stimuli-responsive drug delivery; Postdoctoral Associate at MIT (2015–present), Dr. Michael S. Strano, Label-free single wall carbon nanotube microarray for protein detection and profiling.

<https://www.linkedin.com/in/juyaodong>

My research scope is on synthesizing and optimizing nano materials for biomedical use, such as molecular sensing and therapeutic delivery. More specifically, my Ph.D. work focuses on functionalized mesoporous silica nanoparticles for controlled delivery, especially on the integration with magnetic and upconversion nanocrystals. I am interested in both optimizing biological performances and studying fundamental spectroscopic properties. My postdoc research emphasizes fluorescent carbon nanotube facilitated biomolecular recognition, and multiplexing various detection capacity into a microarray, for diagnosis and product control purposes. I have taught undergraduate courses and mentored both undergraduate and graduate students. Ideally, I would like to teach and direct research at a doctoral university. I am also open to regional comprehensive and four-year undergraduate universities.

ANYL, INOR, COLL, PHYS

Abstract Title: [Label-free optical biomolecular sensing using single wall carbon nanotubes](#)

4. Donald (Donny) A. Robinson, Dept. of Chemistry, University of Utah, 315 S. 1400 E., Salt Lake City, UT 84112. Donny.Robinson@utah.edu; Georgia State University (B.S., 2010; M.S., 2012), Dr. Gangli Wang; The University of Texas at Austin (Ph.D., 2016), Dr. Keith J. Stevenson and Dr. Richard M. Crooks, Tailored functional colloids and interfaces for nanoparticle impact electroanalysis; Postdoctoral Research Assistant at The University of Utah (2013–present), Dr. Henry S. White, Collisional dynamics of electrode reactions with nanoparticles. Professional Developmental Award, UT–Austin, 2015; “Nano-Night” Best Graduate Student Poster, UT–Austin, 2014; Electrochemical Society Outstanding Student Chapter Award, UT–Austin, 2014 (Vice-President, shared); Molecular Basis of Disease Summer Fellowship, GSU, 2010; Outstanding Research at the Undergraduate Level, GSU, 2010.

<https://www.linkedin.com/in/donnyarobinson/>

<https://scholar.google.com/citations?user=pdUTIY4AAAAJ>

I investigate single-nanoparticle interactions with electrode interfaces and the design of multifunctional nanoparticles. My Ph.D. research involved the synthesis of bifunctional Pt-Fe₃O₄ colloids for efficient magnetic capture and detection of biomolecules by electrocatalytic amplification. I am currently studying the nanoscopic dynamic motion of nanoparticles undergoing electrode reactions. In grad school, I served as a TA for 7 semesters and as a research mentor for 4 undergraduate students and 1 high school student participating in a summer fellowship. Most of these students earned authorships on publications. Before entering graduate school, I was oriented toward a research career in the government sector. My experiences educating, training, and advising students have inspired me to instead pursue a professorship at a Ph.D.-granting research institution.

ANYL, COLL, PHYS, INOR, CATL

Abstract Title: [*Effect of solution viscosity on multi-electron transfer from repeated collisions of a single Ag nanoparticle on an Au electrode*](#)

5. Ornella Sathoud, 151 Thorn Ln., Apt 1, Newark, DE 19711. Osathoud@udel.edu, 203-725-5453; Western Connecticut State University (B.A., 2010), Dr. Yuan Mei-Ratliff (Anyl), Assessment of using an ion exchange resin for chromium speciation at ultra-trace concentrations; University of Delaware (Ph.D., 2017), Dr. Karl Booksh (Anyl), (1) Electrokinetic surface plasmon resonance biosensors for point-of-care testing, (2) Designing food analysis experiments for the promotion of critical thinking in the instrumental analysis laboratory. University of Delaware Nanofabrication seed grant (2017), Graduate Scholars Fellowship Award (2012), Sigma XI Undergraduate Research Award (2010); Merit Scholarship for Academic Achievement (2009).

My Ph.D. thesis focused on biosensor fabrication and its characterization, which guided my current interest toward the development of sensors with an agricultural application. A parallel interest is to develop laboratory projects to meet the students' academic needs, but also to provide them with enough exposure to acquire the necessary skills to navigate the changing job market. I taught a wide range of laboratory classes (freshmen through senior) during my graduate studies and developed a set of laboratory experiments for a senior chemistry course: Instrumental Analysis. I mentored five undergraduates, among whom three worked on projects I personally redesigned and directed. I'm interested in teaching and directing undergraduate (and perhaps M.S.) students' research at a four-year college or regional comprehensive university.

ANYL

Abstract Title: [*Designing food analysis experiments for the promotion of critical thinking in the instrumental analysis laboratory*](#)

6. Khanh-Hoa Tran-Ba, Dept. of Chemistry, Columbia University, 634 Havemeyer Hall, New York, NY, 10027. kt2596@columbia.edu; Justus-Liebig University Giessen, Germany (B.S., 2008), Prof. Jurgen Janek, Electrochemical behavior of dissolved metal salts in an ionic liquid; Kansas State University (Ph.D., 2015), Profs. Takashi Ito and Daniel A. Higgins, Single-molecule diffusion measurements for material characterization in one-dimensional nanostructured polymer films; Postdoctoral Research Fellow at Columbia University (2015–present), Prof. Laura J. Kaufman, Design and characterization of biopolymer gels for biophysical studies and bioengineering applications. Phi Lambda Upsilon (PLU) Graduate Research Award (2014).

www.sites.google.com/site/khanhhoatranba/home

My future research will focus on the development of synthetic and natural polymer systems for analytical applications, biotechnologies, and fundamental studies. I propose to characterize polymer structure and properties using microscopic, spectroscopic, and bioanalytical methods. Throughout my career, I have been highly involved in teaching and mentoring activities. Thus, I currently seek a position at a four-year college or research university allowing me to both teach and do research.

ANYL, POLY, PHYS, BIOL

Abstract Title: *Novel characterization of block copolymer and biopolymer matrices using fluorescence microscopy methods*

7. Yang Yang, Department of Chemistry, University of Kansas, 1251 Wescoe Hall Dr., 3037 Malott Hall, Lawrence, KS 66045. yangy@ku.edu; Wuhan University, Wuhan, Hubei, China (B.S., 2013); University of Kansas (Ph.D., 2018), Dr. Yong Zeng, Microfluidic immunoassays for protein and exosome profiling towards cancer diagnosis. University Scholarship, Wuhan University (2010–2012).

I specialize in applying analytical chemistry methods, particularly microfluidics, to study early cancer diagnosis. My previous projects focused on isolation and multiplexed detection of exosome towards blood-based ovarian cancer diagnosis by using a microfluidic chip. My current research centers on microfluidic magnetic bead ELISA streamlined with pneumatic valves to achieve fast and wash-free protein detection. This microfluidic chip also holds the potential to isolate other biomolecules, such as exosomes, for downstream study. In addition, I have accumulated abundant pedagogical experience by teaching general chemistry and organic chemistry laboratories at the University of Kansas. I aspire to find a postdoctoral or faculty position to continue my research in a doctoral degree granting university or a research institute.

ANAL, BIOT

Abstract Title: *Microfluidic magnetic bead ELISA streamlined with pneumatic valves*

8. Sara E. S. Martin, Harvard Medical School, HIM 1018D, 77 Avenue Louis Pasteur, Boston, MA 02115. Sara_Martin2@hms.harvard.edu; Lebanon Valley College (B.S., 2009); University of Delaware (Ph.D., Chem and Biochem, 2014), Prof. Donald Watson (Org Synthesis), Development of the silyl-Heck reaction: Preparation of organosilanes via the transition metal-catalyzed silylation of alkenes; NIH Postdoctoral Fellow at Harvard Medical School, (2014–present), Prof. Suzanne Walker, Developing new tools for the study of O-GlcNAc transferase in disease. Ruth L. Kirschstein National Research Service Award (Harvard Medical School, NIH F32, 2016); Elizabeth Dyer Award for Excellence in Teaching (University of Delaware, 2012); NSF Graduate Research Fellowship Program Honorable Mention (2011); Chemistry–Biology Interface Fellow (University of Delaware, NIH T32, 2009–2011).

www.linkedin.com/in/saraesmartin

I am interested in research questions relevant to human health that lie at the interface of chemistry and biology. I am pursuing a faculty position at a primarily undergraduate institution because I enjoy teaching and interacting with undergraduate students in both classroom and research settings. I have experience mentoring undergraduates in the laboratory to achieve technical competence, to take ownership of projects, and to achieve the next step toward their desired careers. I have assisted in general chemistry and biochemistry courses and served as adjunct faculty for a general chemistry lab. The focus of my research will be to develop small molecule chemical probes for glycosyltransferases relevant to bacterial cell wall biosynthesis and to understand their mode of action. Students in my lab will be exposed to a variety of chemical and biological research techniques.

ORGN, BIOL, MEDI

Abstract Title: [Developing new tools for the study of O-GlcNAc transferase in disease](#)

9. Joseph W. Meisel, Dept. of Chemistry, New York University, 100 Washington Square East, Silver Center Floor 10 Box 190. joe.meisel@nyu.edu, 317-702-5631; Indiana University Bloomington (B.S., Biochem, dept. honors, high distinction; B.S. Human Bio, high distinction; Minor, Leadership, Ethics, & Social Action, 2009); University of Missouri-St. Louis (M.S., Org Chem, 2013; Ph.D., Org Chem, 2016), Prof. George W. Gokel, Synthesis and characterization of amphiphiles for mammalian cell transfection and antimicrobial activity; Postdoctoral Associate at New York University Department of Chemistry, (2016–present), Prof. Andrew D. Hamilton, Synthesis of peptidomimetic scaffolds to modulate protein–protein interactions.

www.linkedin.com/in/joseph-meisel

www.researchgate.net/profile/Joseph_Meisel

My goal is independent, interdisciplinary research to design small-molecule peptidomimetics and supramolecular assemblies to modulate protein–protein and protein–membrane interactions, focusing on compounds with translational potential as chemicals tools and drug candidates to study and rectify human diseases, in particular, creating synthetically tractable small molecule scaffolds capable of adopting predictable conformations and displaying functional groups with density and diversity rivaling natural protein epitopes. I'll use organic synthesis, self-assembly, transmembrane transport, antibacterial resistance, and gene delivery to address human disease associated with cellular membranes. I seek a tenure-track position at a Ph.D.-granting institution. My passion for teaching and promoting scientific literacy led me to design and teach a nonmajors course on the chemistry of beer brewing.

ORGN, BIOL, MEDI

Abstract Title MAMBA: [*Hydrogen bond organized beta-strand peptidomimetics*](#)

10. Sarah J. Smith, Dept. of Pharmacy, University of Toronto, 144 College St., Toronto, ON M5S3M2, Canada. Sarahjane.smith@utoronto.ca; Massachusetts Institute of Technology (B.S. Bio; B.S. Chem, 2009); University of California, San Diego (M.S., 2011; Ph.D., 2016), Prof. F. Akif Tezcan, Metal-controlled assembly of peptide and protein-based engineered biomaterials; Postdoctoral Fellow at University of Toronto (2016–present), Professor Shana Kelley, Development of novel electrochemical detection methods for biological targets.

I have an extensive background conducting interdisciplinary research in the fields of biological, inorganic, materials, and analytical chemistry. During my graduate research at UC San Diego with Prof. Akif Tezcan, I studied the use of metal ions to control the secondary, tertiary, and quaternary structures of peptides and proteins. As a postdoctoral fellow at the University of Toronto with Prof. Shana Kelley, I am working on more applied research, developing analytical devices for disease diagnostics using bio-molecular interactions. Both positions have afforded the valuable opportunity to mentor undergraduate and high school students. My research will combine biological and inorganic chemistry to provide new methods for disease diagnostics and therapeutic delivery methods. I hope to teach and to establish a robust research program, likely at a M.S. degree- or Ph.D.-granting school.

BIOL, INOR

Abstract Title: *Incorporation of synthetic, toe-hold based gene circuits for the development of electrochemical sensors for rapid disease diagnostics*

11. Gregory R. Wiedman, Public Health Research Institute, Rutgers New Jersey Medical School, 225 Warren St., Newark, NJ 07103. grw44@njms.rutgers.edu; University of Pennsylvania (B.S.E., M.S.E., 2010), Dr. Bohdana Discher (Biochem and Biophysics), Concentrations in bioengineering and nanotechnology; Johns Hopkins University (PhD., 2015), Dr. Kalina Hristova (Mat Sci, Biophysics), Developing membrane active peptides for endosomal escape of macromolecules; Public Health Research Institute Rutgers NJ Medical School (2015–present), Dr. David S. Perlin, Designing biosensors of small molecules for clinical applications and microbiology studies.

<https://www.linkedin.com/in/gregory-wiedman-766676a4/>

<https://molecularyoga.wordpress.com/>

I study how molecules evolve. I do this to develop both practical applications and a better understanding of how molecules can be rationally designed. My work draws on my multidisciplinary background in biochemistry, biophysics, and materials science engineering. I use established methods such as fluorescent microscopy, mass spectroscopy, and cell culturing. I also strive to include emerging techniques like electrical impedance spectroscopy and nanodevices. I am deeply committed to improving science literacy through both professional teaching and volunteer outreach programs. I believe in the idea of teaching as research; I use data from my classroom to help me better instruct my students. My goal is to start a research program at a highly active research university. I hope this program can also promote public involvement in research and make learning about science fun and exciting again.

BIOL, BIOT, MEDI, ANYL

Abstract Title: *Molecular Yoga: The juxtaposition of rational design and synthetic molecular evolution to create new, useful molecules*

12. A. Tuley, College of Pharmacy, The University of Texas at Austin, 107 W. Dean Keeton St, Austin, Tx 78712. alfred.tuley@utexas.edu; Texas A&M University – Corpus Christi (B.S. Chemistry, 2009), Biochemistry emphasis; Texas A&M University – College Station (Ph.D. Chemistry, 2015), Prof. Wenshe Liu, “Expanding the Genetic Code to Probe Biological Systems”; NIH-IRACDA Postdoctoral Fellow at the University of Texas at Austin (2015-present); Prof. Walter Fast, Synthesis of covalent enzyme inhibitors; NCI Research Supplement to Promote Diversity in Health-Related Research (2013-2015)
<https://www.linkedin.com/in/alfredtuley/>
<https://scholar.google.com/citations?user=E5adtUoAAAAJ&hl=en&oi=ao>

I am primarily interested in studying covalent protein modifications through the development of novel inhibitors and bioorthogonal reagents. For my independent career, I would like to utilize my experience in chemical biology to continue studying protein modifications that could expand the current toolkit available to biologists. I have been actively involved in mentoring undergraduate researchers, and would prefer a career at a primarily undergraduate institution (PUI). In addition to my research interests, I have also held part-time teaching appointments at Southwestern University, a small liberal arts college that emphasizes active learning pedagogy. I am passionate about training an informed citizenry and wish to find a position where I can continue educating undergraduate students.

BIOL, ORGN

Abstract Title: [*Derivatization of halopyridines for covalent enzyme inhibition*](#)

13. Hazim Al-Zubaidi, Dept. of Chemistry, Western Michigan University, 1903 W. Michigan Ave., Kalamazoo, MI 49008-5413. hazimabdulrazz.alzubaidi@wmich.edu; Al-Nahrain University (B.S., 2003; M.S., Anyl Chem, 2006), Dr. Shahbaz A. Maki, Water quality in some Iraqi water resources; Western Michigan University (Ph.D., Inorg Chem, 2017), Dr. Sherine Obare, Selective catalysts for conversion of biomaterials into commodity chemicals.

My research focuses on analytical and inorganic chem, with 5+ years' design, synthesis, characterization, and use of metallic, multi-metallic, metal oxide, and semiconductor nanoparticles for catalytic applications. Synthetic approaches developed environmentally friendly procedures. Nanoparticles mediated reactions to advance converting biomass into fuels and commodity chemicals and remediated toxic environmental contaminants. My research appeared in peer-review manuscripts and at national meetings. Given a Certificate of Merit by ACS Environmental Chem Div and a University award for Excellence in Research and Creative Scholarship. I have 10+ years of teaching general, organic, inorganic, and analytical chem and 5+ years of mentoring undergrads and high school students in research. I'd like to teach undergrads, engaging them in environmental chem research and enhancing their success.

CATL, ENVR, INOR, ANYL

Abstract Title: *Rationally Designed nanoscale catalysts for green transformations to form commodity chemicals*

14. Monique Shauntá Wilburn, Dept. of Chemical Engineering, University of Virginia, Charlottesville, VA. monique.wilburn1@yahoo.com; The Pennsylvania State University (B.S., Aerospace Eng, 2004); Power Systems and Space Suit Systems Engineer at NASA Johnson Space Center, (2004–2017), Dr. Eric Darcy, Development of Li-ion battery cell manufacturing defect detection and prevention methods as well as General battery system safety characterization and Design techniques for space vehicles and astronaut life support systems; University of Houston (Ph.D., Chem Eng, 2016), Dr. William Epling, Methane oxidation over, and sulfur interactions with, Pd/Pt bimetallic catalysts; Postdoctoral Research Associate at University of Virginia (2017–present), Dr. William Epling, Automobile engine exhaust aftertreatment systems for emissions reduction. Rotary Stellar Individual Award Nominee for Contributions to Battery Technology Development, NASA Technical Excellence Awards for Contributions to Space Exploration, NASA Early Career Medal for Outstanding Leadership, NASA Academic Fellowship, Dow Chemical Building Engineering & Science Talent Symposium Participant.

By leveraging my NASA and academic research experience, I will create an interdisciplinary laboratory for catalysis research as it relates to emissions abatement, developing thermally stable and robust battery cell materials in an effort to help cell manufacturers reduce their failure rates, and development of environmentally friendly chemical processes and battery materials. I have a particular interest in teaching reaction engineering and transport courses as well as electives pertaining to chemical process safety and engineering ethics. By fostering a challenging but nurturing learning environment at a research-focused university, I will be a professor who can use her laboratory not only to nourish her scientific curiosity and impact society but also to better prepare students to be professional, ethical, motivated, and diversely skilled researchers and engineers.

CATL

Abstract Title: *Sulfur interactions with bimetallic Pd/Pt catalysts*

15. Ximing Zhang, 500 Central Dr., Room 336, West Lafayette, IN 47906.
zhan1290@purdue.edu, 919-534-5188; Purdue University (Ph.D., Ag and Bio Engineering, 2015); Postdoctoral Researcher at the Laboratory of Renewable Resources Engineering (LORRE; 2015–present).

I focus on advanced, low-cost green processes to address outstanding issues in lignocellulosics conversion. Collaborating at Purdue University's Center for Catalytic Conversion of Biomass to Biofuels (C3Bio), I explore lignin-carbohydrate interfaces among chemistry, catalysis, and biology. I'm developing a research program for developing new transformations and molecules that can synthesize advanced biomaterials and key chemical intermediates using thermochemical methods. I've contributed to elucidating biomimetic catalyst reaction mechanisms for carbohydrate conversion to value-added chemicals and understanding lignin-aided ozonolysis for cellulose surface modification. My background in bioproducts and catalysis provides a good foundation for a research program. I want to teach undergrad and grad classes. I find teaching and advising enriching and rewarding and look forward to teaching.

CATL, CARB, ENVR, FUEL

Abstract Title: [*Maleic acid and aluminum chloride catalyzed conversion of glucose to 5-\(Hydroxymethyl\) furfural and levulinic acid in aqueous media*](#)

16. Shiqiang Zhuang, Dept. of Mechanical Engineering, New Jersey Institute of Technology, 200 Central Ave., Newark, NJ 07032. sz86@njit.edu; University of Science and Technology of China (A.B., 2008); New Jersey Institute of Technology (M.S., 2013); New Jersey Institute of Technology (2014–present), Dr. Eon Soo Lee (ME), Innovative low-cost and high-performance nano-graphene-based catalysts for oxygen reduction reaction. Grants: 2016 NJIT Faculty Seed Grant; Fall 2015 NSF I-Corps Site at NJIT; Spring 2015 NSF I-Corps Site at NJIT; Award: 2017 Dana Knox Student Research Showcase Awardees.

https://www.researchgate.net/profile/Shiqiang_Zhuang

I am interested in the investigation of graphene-based catalyst for oxygen reduction reaction applications such as fuel cells. I hope to interest students in catalyst, catalysis, and fuel cell technology in this research. I have strong experience on physical and chemical characterizations. I want to teach and direct the research of graduate students at a regional comprehensive university.

CATL

Abstract Title: [*Metal organic framework-modified graphene-based catalyst for oxygen reduction reaction*](#)

17. Junyang Xian, Dept. of Chemistry, Drexel University, 3141 Chestnut St., Philadelphia, PA 19104. jx55@drexel.edu., Office: 215-895-2647, Cell: 215-301-8037; Hefei University of Technology (B.S., 2009), B.S. Thesis, College of Pharmacy, Nankai University, Extraction and purification of enzyme; University of Science and Technology of China (M.S., Phys. Chem., 2012), Weixin Huang, Synthesis of size-controlled PVP-capped palladium nanoparticles, and size-specific catalytic activity of PVP–Pd for benzyl alcohol oxidation in water; Drexel University (Ph.D., Chem. Ed., 2017), Dr. Daniel King, The effects of several teaching techniques on student performance and The effectiveness of LEGO activities on students' understanding of chemical kinetics and equilibrium.

My first research interest is developing effective teaching techniques to help students improve their understanding of chemistry. My second research interest is analyzing the effects of existing teaching techniques on student performance. I have five years of experience as a teaching assistant at Drexel University. I taught general chemistry labs and recitations in each year. I love teaching as a teaching assistant and I am looking for a teaching position in universities or colleges. I am also interested in a tenure-track position in the research of chemical education or STEM education.

CHED

Abstract Title: [*Using LEGO[®] to help students understand kinetics and equilibrium concepts*](#)

18. Swarnapali De Silva Indrasekara, Fitzpatrick Institute for Photonics, Dept. of Biomedical Engineering, Duke University, P.O. Box 90281, Durham, NC, 27708. ad314@duke.edu, a.pali.dsi@gmail.com; University of Peradeniya (B.S., 1st class honors—equivalent to summa cum laude, 2008); Rutgers University, New Brunswick, NJ (Ph.D., 2014), Dr. Laura Fabris, Fabrication of nanomaterials for enhanced vibrational spectroscopies; Postdoctoral Associate at Rice University (2014–2016), Dr. Christy F. Landes, Single molecule spectroscopy of nanomaterials; Postdoctoral Associate at Duke University (2016–present), Dr. Tuan Vo-Dinh, Nanomaterials for enhanced biosensing and therapy. Finalist: Bioanalysis New Investigator Award—decisions currently underway (2017); Dean’s Research Excellence Award, Rutgers University, NJ—awarded only to three graduate students (2014); SPIE Research Excellence Award, SPIE & Newport Corporation (2013); Dennis W. Wertz Award for Excellence in Teaching, North Carolina State University, NC—awarded to only 2 graduate teaching assistants out of 25 (2010).

<https://paliindrasekara.wordpress.com>

I plan to apply for tenure-track faculty positions in Ph.D.-granting universities. Based on my interdisciplinary research that lies at the intersection of nanotechnology, analytical chemistry, and medicine, I intend to apply for positions in the department of chemistry, materials, and biomedical engineering. To date, my research contributions have been two-faceted; rational design and fabrication of inorganic nanomaterials, and spectroscopic interrogation of processes occur at nanoparticle interfaces for effective analytical and biomedical applications. My goal is to establish my own lab that uses nanoscale engineering and optical vibrational spectroscopy as tools to innovate new technologies to understand molecular level processes significant in molecular biology, medicine, and catalysis, and also to develop translational technologies for sustainable living and improved global health.

ANYL, COLL, INOR, PHYS

Abstract Title: [*Nanoscale engineering for fundamental biophysical studies and biomedical applications*](#)

19. Yuan Lyu, Dept. of Agricultural and Biological Engineering, Purdue University, 225 South University St., West Lafayette, IN 47906. lv10@purdue.edu; East China Normal University (M.S., 2013), Dr. Zhongyi Chang, Food chemistry and food processing; Purdue University (Ph.D., 2017), Dr. Ganesan Narsimhan, Investigation of interaction between antimicrobial peptide from natural resources and cell membrane using molecular dynamics simulation and experiment.

https://www.researchgate.net/profile/Yuan_Lyu5

I am interested in protein interactions with cell membranes and propose to characterize their self-assembling property and function in the human body environment through molecular dynamics simulation and biochemical techniques. I hope to interest students in applying biochemistry and engineering in this research. I assisted in Thermodynamics and Transport Operations courses. I would like to teach and direct the research of undergraduate students at a four-year college or regional comprehensive university.

BIOL, ANYL

Abstract Title: [*Potential of mean force for insertion of antimicrobial peptide melittin into a pore in mixed DOPC/DOPG lipid bilayer by molecular dynamics simulation*](#)

20. Katherine R. Phillips, 586 Winthrop Mail Center, Cambridge, MA 02138. kphill@mit.edu; Brown University, (Sc.B., Chem and Math, 2010); Harvard University, (M.A., 2013; Ph.D., 2016), Dr. Joanna Aizenberg, Sol-gel chemistry of inverse opals; Postdoctoral Researcher at Massachusetts Institute of Technology (2016–2017), Dr. Yang Shao-Horn, Developing novel electroreduction catalysts for carbon dioxide conversion; Postdoctoral Researcher at Massachusetts Institute of Technology (2017–present), Dr. T. Alan Hatton, Electrochemical carbon dioxide capture. NSF graduate research fellowship, DOD National Defense Science and Engineering Graduate fellowship.

<https://www.linkedin.com/in/katherine-phillips-a9441611/>

I am interested in developing novel materials to solve big energy and environmental problems, and to date I have studied colloidal assembly, nanomaterials synthesis, and electrochemistry, with energy and environmental applications in mind. I believe that one of the benefits of applied research is that it can help motivate students to study chemistry, something I have tried to incorporate into the variety of chemistry courses I have taught. In the future, I hope to teach coursework and mentor research for undergraduate and graduate students at a research university while pursuing nanomaterials research for fundamental and applied studies.

COLL

Abstract Title: [*Self-assembly and applications of inverse opals*](#)

21. Prahlad K. Routh, Dept. of Physics, Columbia University, 538 West 120th St., New York, NY, 10027. pr2538@columbia.edu; Indian Institute of Technology Madras, Chennai, India (B.Tech., 2009); State University of New York at Stony Brook (M.S., 2013; Ph.D., 2016), Dr. Mircea Cotlet, and Dr. T. A. Venkatesh, Water based self-assembly of conjugated polymer/nanocomposite thin films: Controlling morphology and optical properties. Best Poster Award, Advanced Energy Conference (AEC), Albany, NY (2014); Research Foundation Seed Grant, Stony Brook University, Stony Brook, NY (2011); Student Scholarship Award, NSLS-II & CFN Users' Meeting, BNL, Upton NY (2016).

My research interests are evaluating electronic and optical properties of advanced materials such as perovskites, 2-D materials and their heterostructures for solar energy and nano-engineered electronic devices applications using ultrafast photodynamic characterization tools. My graduate research has focused on single molecule spectroscopy techniques to study organic and inorganic hybrid nanomaterials. My teaching responsibilities include development and seminar based discourse of a core course, "Frontiers of Science," focusing on developing scientific habits of mind and emphasizing recent developments in neuroscience, physics, biodiversity, and earth science. I look forward to applying my research and teaching skills at a university where I can teach undergraduate courses and mentor grad and undergrad research in opto-electronic structure property characterization of advanced materials.

ANYL, INOR

Abstract Title: [*Photoinduced single nanocrystal study of hybrid semiconducting nanomaterials*](#)

22. Shruti Sharma, Dept. of Materials Science and Chemical Engineering, Stony Brook University, 700 Health Sc. Dr., Chapin Apt. MB502, Stony Brook, NY 11790.
shruti.sharma@stonybrook.edu; Stony Brook University (M.S., 2015; Ph.D., anticipated 2018), Dr. Rina Tannenbaum, Geometry driven properties of carbon nanomaterials for cancer applications.
www.linkedin.com/in/shrutisharmasbu

I seek a joint career in nanomaterials research and STEM teaching and outreach. I complement my Ph.D. with experiential learning methods such as STEM outreach to gain mentoring and pedagogical skills. I've conceptualized and guided research modules for high school and undergrad students and co-conducted a middle school hands-on biochemistry module. As a TA I've led project discussions and conducted tutorials for concepts in materials science and chemical engineering. My research focuses on synthesizing and characterizing carbon-based hybrid nanomaterials. I'm interested in exploring their multi-modal biomedical applications for cancer drug delivery, imaging, and therapeutic capabilities. I'm interested in making and studying novel nanomaterials systems, making these studies more accessible to students at all levels through video tutorials, hands-on activity kits, and educational modules.

COLL

Abstract Title: *Metal nanoparticle decorated meso-graphene oxide composites as theranostics*

23. Tharanga K. Wijethunga, Dept. of Chemical Engineering, Massachusetts Institute of Technology, E19-536, 77 Massachusetts Ave., Cambridge, MA, 02139. tharanga@mit.edu; University of Colombo, Colombo, Sri Lanka (B.S., Special Degree in Chem, 2010); Kansas State University, Manhattan, KS (Ph.D., 2015), Prof. Christer B. Aakeröy, Hydrogen- and halogen-bond driven co-crystallizations: From fundamental supramolecular chemistry to practical materials science; Postdoctoral Associate at Massachusetts Institute of Technology, Cambridge, MA (2016–present), Prof. Bernhardt L. Trout and Prof. Allan S. Myerson, Heterogenous nucleation of small molecular pharmaceuticals.

<https://www.linkedin.com/in/tharanga-k-wijethunga/>

https://www.researchgate.net/profile/Tharanga_Wijethunga

My research interests are in the areas of co-crystals and applications, co-crystal polymorphism, polymorphism of pharmaceuticals, heterogeneous nucleation and epitaxy, supramolecular polymers, and design and synthesis of novel hydrogen and halogen bond donors and acceptors. I am currently using the concepts of molecular epitaxy to design effective crystalline heteronucleants to enhance the nucleation and growth kinetics of active pharmaceutical ingredients (APIs). I have a Kaufman Teaching Certificate from MIT; it and the Graduate TA Professional Development program at Kansas State exposed me to evidence-based teaching methods. I am interested in teaching inorganic chemistry, supramolecular chemistry, crystal engineering, organic chemistry, and materials chemistry. I am interested in teaching and conducting research in a Ph.D. institution, comprehensive university, or four-year college.

COLL

Abstract Title: [Design of crystalline heterosurfaces for direct nucleation of active pharmaceutical ingredients](#)

24. Trent E. Balias, Dept. of Pharmaceutical Chemistry; University of California, San Francisco, 1700 4th St., Box 2550, San Francisco, CA 94158. trent.balias@gmail.com; The University of Pittsburgh at Greensburg (UPG) (B.S., Applied Math, 2006); Stony Brook University (SBU) (Ph.D., Applied Math & Computational Bio, 2012), Dr. Robert C. Rizzo, Application and development of computational tools in drug discovery: Docking method development and molecular dynamics simulation; Postdoctoral Scholar at University of California, San Francisco (UCSF) (2012–present), Dr Brian K. Shoichet, Developing docking methods to aid in ligand discovery. Graduated Summa Cum Laude from UPG (2006); NIH National Research Service Award predoctoral fellowship (F31CA134201) at SBU (2008–2012); President’s Award to Distinguished Doctoral Student from SBU (2012); NIH National Research Service Award postdoctoral fellowship (F32 GM108161) at UCSF (2014–2015).

<http://docking.org/~tbalias>

<https://www.linkedin.com/in/trent-balias-05250097>

Trent is a computational biologist whose research focuses on developing and using computational methods to improve therapeutics. During his postdoctoral and graduate studies, Trent developed new docking methods for ligand discovery, while using molecular dynamics to understand the role water plays in the binding event and drug resistance. He has coauthored over 11 research articles. Trent cares deeply about mentoring and teaching science. As a postdoc, Trent mentored two graduate students. His teaching experience includes being a teaching assistant for calculus 1 and 2, as well as giving several guest lectures in a course on computational biology and drug discovery and running tutorials in a molecular simulation computer lab. Trent’s goal is to obtain a faculty position at a university where he will continue his research and teaching in computational methods for drug discovery.

COMP, MEDI, PHYS

Abstract Title: [Developing and applying computational approaches in early-stage drug discovery](#)

25. Duminda S. Ranasinghe, Quantum Theory Project, Dept. of Chemistry, University of Florida, FL 32601. dranasinghe@chem.ufl.edu; Institute of Chemistry Ceylon, Sri Lanka and University of Kelaniya, Sri Lanka, (B.S., 2009); Wesleyan University (Ph.D., 2015), Prof. George A. Petersson, The development of the CBS-Wes Method; Postdoctoral Associate at University of Florida (2015–present), Prof. Rodney J. Bartlett, Using the power of exact conditions to develop density functionals.

<https://dranasinghe.wordpress.com/>

During my Ph.D. candidacy, I devised innovative ways to reduce computational cost by calculating core-valence correlation energy using (density functional theory) DFT. My method reduces computational cost, which can be hours to seconds, which is greatly beneficial for large molecular systems, mainly organic materials. Currently, I am working as a postdoctoral associate at the University of Florida, where I am continuing to develop new functionals using exact conditions in chemistry and physics. I have worked as teaching assistant in general chemistry laboratory and physical chemistry courses. My experiences at Wesleyan University draw my attention towards PUI that encourage undergraduate research. I would like to teach Physical Chemistry I and II, along with laboratory courses, augmenting computational chemistry into course material.

PHYS, COMP

Abstract Title: [*Power of exact using conditions to develop density functionals*](#)

26. Natalia Sizochenko, Interdisciplinary Center for Nanotoxicity, Jackson State University, MS. sizochenko@icnanotox.org, +1-323-507-8976; Odessa National University (Ukraine; B.S., Chem, specialization—Org Chem, minor—Education, 2010); Odessa National University (Ukraine; M.Sc., Chem, specialization—Org Chem, 2011), Dr. Victor Kuz'min, Comparative QSAR analysis of toxicity and mutagenicity of organic compounds of different classes; University of Gdansk, Poland (Ph.D., 2016), Dr. Tomasz Puzyn, Optimal selection of descriptors for structure-activity modeling of nanoparticles based on causality analysis; Research Associate (2015–2016), Dr. Jerzy Leszczynski, Computational modeling on nanoparticles; Research Associate at Jackson State University (2016–present), Dr. Jerzy Leszczynski, Quantum chemical simulations, molecular docking and QSAR of disease-related proteins.

In my Ph.D. dissertation I focused mainly on predictive nanotoxicology. In addition to this expertise, I gained other skills. I have recently developed a multi-level project studying ligand binding and reactivity for anti-tubercular therapy, which combines quantum chemical ONIOM modeling, docking, and QSAR studies. I find this exciting; modeling at different levels allows you to understand the nature of processes better. I already have a great track record with mentoring. Two of my students recently defended their Ph.D. dissertations and one M.S. will graduate soon. One once-poorly motivated student completed 2 projects and got 2 peer-reviewed articles accepted in 15 months. I've developed a grad course in applications of computational chemistry methods. This course is now part of the comprehensive exam at Jackson State. I want to teach any level students, high school to grad school.

COMP, MEDI

Abstract Title: [*Deep learning vs Zika virus: At the crossroads of computational chemistry, systems biology, data mining and computer science*](#)

27. Liang Zheng Tan, Dept. of Chemistry, University of Pennsylvania, 231 S. 34 St., Philadelphia, PA 19104-6323. liangtan@sas.upenn.edu; California Institute of Technology, Pasadena (B.S., Physics, 2008); University of California, Berkeley (Ph.D., Physics, 2014), Prof. Steven G. Louie, Electronic and vibrational properties of two-dimensional materials constructed from graphene and molecular components; Postdoctoral Fellow at Dept. of Chemistry, University of Pennsylvania (2014–present), Prof. Andrew M. Rappe, Photovoltaic and nonlinear optical effects in the solid state and in molecules.

<http://lztan.github.io>

<https://scholar.google.com/citations?user=qQLD2zkAAAAJ>

I am interested in the interaction of light with matter, including photocurrent generation and nonlinear optical effects such as optical rectification and sum frequency generation. In particular, I wish to understand the fundamental physical limits governing such optical processes. My research is driven by the goal of placing theoretical upper bounds on materials performance that apply across materials classes and of refining these bounds according to specific materials classes. I make use of density functional theory (DFT) as well as post-DFT and high-throughput methods. I enjoy seeing theory tested against—and informed by—experiment, and I would like to establish a research group at a Ph.D.-granting research university.

PHYS, COMP

Abstract Title: [Pushing nonlinear spectroscopy to its limit: Theoretical upper bounds for second harmonic generation in molecules and materials](#)

28. Alexander C. Davis, Dept. of Chemistry, Franklin and Marshall College, 415 Harrisburg Ave, Lancaster, PA 17603. alex.davis@fandm.edu; Purdue University (B.S. Environmental Chemistry 2001, B.S. Biochemistry 2001); University of Western Australia (M.S. Chemistry 2005), Dr. Allan McKinley, Effects of acidity on bacterial sulfate reduction and metal bioprecipitation in acid rock drainage groundwater using three different carbon sources; Purdue University (Ph.D. Chemistry 2011), Dr. Joseph S. Francisco, Ab initio study of chain branching reactions in the combustion and atmospheric degradation mechanisms of hydrocarbons; Postdoctoral Research Assistant at the National Institute of Science and Technology (2013-2015), Dr. Jeffrey Manion, Shock tube and computational investigation of second generation biofuel combustion kinetics; Visiting Assistant Professor at Franklin and Marshall College (2015-Present), The atmospheric oxidation and combustion mechanisms of unsaturated hydrocarbons and oxygenated species; National Research Council Research Associate Fellowship (2013-2015)

<https://sites.google.com/a/fandm.edu/davis-research-group/>

I am interested in the integration of computational resources into the field of chemistry. My research group (currently six undergraduates) at Franklin and Marshall college uses computational chemistry to study a wide range of topics, including the oxidation of hydrocarbons under atmospheric and combustion conditions, the mechanism of antioxidants, the Diels-Alder reaction involving aromatic species, and the development of inexpensive instrumentation for use in undergraduate labs. As a result, my current and future work spans several disciplines. I have developed and taught upper level undergraduate courses in kinetics and thermodynamics and atmospheric chemistry as well as general chemistry for the past two years. I seek a tenure-track position at a primarily undergraduate institution or small to medium sized Ph.D. granting university.

ANYL, CHED, COMP, ENVR, ORGN, PHYS

Abstract Title: [Computational study of ketoheptylperoxy radical atmospheric decomposition and combustion](#)

29. A. Aneksampant

Abstract Title: [Microbial effect of iron from hematite into seawater mediated via anthraquinone-2,7-disulfonate](#)

30. Craig Warren Davis, Dept. of Civil, Environmental, & Geo-Engineering, University of Minnesota, 500 Pillsbury Dr. SE, Minneapolis, MN 55455. davi3148@umn.edu; University of Delaware (B.S., Civil & Envr Eng, Distinction, 2011); University of Delaware (Ph.D., 2016), Dr. Dominic M. Di Toro (Civil & Envr Eng), Predicting the fate and transport of organic contaminants using quantum-chemically estimated poly-parameter LFER/QSAR descriptors; Postdoctoral Research Associate at University of Minnesota (2016–present), Dr. William A. Arnold, Resource recovery / Bio-hydrogen production from high strength wastewater using composite-coated encapsulated bacteria. Eugene M. Du Pont Memorial Scholarship, University of Delaware (2007–2011,); Imperial College Summer Exchange Scholar, Imperial College, UK (2011); Department of Education GAANN Fellowship, University of Delaware (2012–2015); Carl J. Storm Underrepresented Travel Award, Gordon Research Conference (2014).

<https://www.linkedin.com/in/craig-davis-48702918/>

I am interested in predicting the fate, transport, and toxicity of novel charged organic contaminants in environmentally relevant systems using quantum chemistry and molecular dynamics. Additionally, I am interested in elucidating the biodegradability of novel ionic species (e.g., ionic liquids) and developing predictive QSAR/pp-LFER models for nonequilibrium environmental processes. I have published my work in *Environmental Science & Technology* as well as *Chemosphere*. I have assisted in teaching courses in fate and transport at the undergraduate and graduate levels. Additionally, I have designed and taught a course on adsorption theory and modeling at the graduate level. I wish to conduct research, teach, and direct graduate student research at a major research university in the United States.

ENVR, COMP, AGRO, TOXI

Abstract Title: *Predicting solvent-water partitioning of charged organic species using quantum-chemically estimated Abraham pp-LFER solute parameters*

31. Niluka Dissanayake, Dept. of Chemistry, 1903 W. Michigan Ave., Kalamazoo, MI 49008-5413. nilukamadhumi.m.dissanayake@wmich.edu, 269-290-9360; University of Peradeniya, Sri Lanka (B.S., 2009; M.Phil., Anyl Chem, 2014), Dr. M. Y. Udugala-Ganehenege, Synthesis of macrocyclic complexes for the electrochemical reduction of carbon dioxide; Western Michigan University (Ph.D., anticipated Dec 2017), Dr. Sherine O. Obare, Strategies to elucidate the stability and toxicity of nanoparticles exposed to various environmental contaminants.

An inorganic and environmental chemist, I will establish a research program bridging both. I've synthesized and characterized macrocyclic complexes and nanoscale materials (metals, metal oxides, semiconductors) for electrochemical reduction of carbon dioxide and detecting toxic organic pesticides, respectively. Analytical skills comprise electrochemistry, electron microscopy, optical spectroscopy, and mass spectrometry. I've used my experience in toxicology to investigate the environmental impact of anthropogenic nanoparticles. My molecular biology techniques include cell culture, ELISA, and methods to study DNA damage. I've taught lectures and labs in general, organic, and inorganic chem. I will provide interdisciplinary research experiences to excite students to pursue chemistry. My experience will allow me to teach traditional chemistry courses and develop new interdisciplinary ones.

ENVR, TOXI, INOR, ANYL

Abstract Title: *Elucidating mechanisms of toxicity of nanoparticles exposed to various environmental factors*

32. Alison R. Kennicutt, 3301 Colerain Ave., Apt 204, Cincinnati, OH 45225.
akennicutt@gmail.com, 518-852-5287; Rensselaer Polytechnic Institute, (B.S., Civil Eng, 2009; M. Eng., Environmental Eng, 2011; Ph.D., Environmental Eng, 2015), Dr. James E. (Chip) Kilduff, Computational chemistry approaches to evaluating drinking water treatment processes for emerging contaminants; Postdoctoral Research Associate via the National Research Council Research Associate Program at U.S. Environmental Protection Agency (2015–2018), Dr. Jonathan G. Pressman, Dr. David G. Wahman, and Dr. Susan Glassmeyer; Chloramination of natural organic matter in concentrated drinking water for disinfection byproduct mixtures research.

<https://www.linkedin.com/in/alison-kennicutt-10b4a645/>

My graduate and postdoctoral work has been focused on water quality and water treatment—I have a background in activated carbon adsorption, membrane filtration, chlorine and chloramine oxidation, as well as computational chemical modeling. As a faculty member, I would like to provide a focus on environmental engineering/science and the issues surrounding environmental health. I would like to inspire students to pursue scientific inquiry, as both professionals and responsible members of society. I have previously assisted in courses focused on statics and material properties, which is when I fell in love with teaching. I am interested in teaching both core and more specified courses at the undergraduate and graduate levels as well as guiding research for undergraduate, master's degree, and possibly doctoral degree students.

ENVR

Abstract Title: *Preparation of chloraminated concentrated drinking water for disinfection by-product mixtures research*

33. Carrie A. McDonough, Dept. of Civil & Environmental Engineering, Colorado School of Mines, 1012 14th Street, Coolbaugh Hall, Golden, CO 80401. carrie.a.mcd@gmail.com, 216-832-8932; Massachusetts Institute of Technology (B.S., 2008); University of Rhode Island Graduate School of Oceanography (Ph.D., 2017), Dr. Rainer Lohmann (Oceanography), Spatial distribution, air-water exchange, and toxicity of organic pollutants using passive samplers; Postdoctoral Fellow at Colorado School of Mines (2017–present), Dr. Christopher Higgins, Using high-resolution mass spectrometry to investigate environmental fate and bioaccumulation of per- and polyfluoroalkyl substances (PFASs) from aqueous film forming foams. ACS C. Ellen Gonter Environmental Chemistry Paper Award, 2017; University of Rhode Island Research and Scholarship Excellence Award, 2017; Hudson River Foundation Mark B. Bain Graduate Fellowship, 2016–2017; University of Rhode Island Graduate School Fellowship, 2016–2017; ACS Graduate Student Award in Environmental Chemistry, 2016.

carriemcdonough.com

My research goal is to apply my extensive experience in analytical chemistry to investigate the fate of persistent anthropogenic chemicals in the environment, including pathways for human exposure and effects on human health. I have mentored several undergraduate students and served as a teaching assistant as well as a guest lecturer. I am prepared to lead courses in analytical chemistry, environmental chemistry, marine pollution, and general chemistry, and have a passion for including writing, communication, and public outreach within my courses. I seek a tenure-track faculty position at a doctorate-granting research university where I can lead an ambitious research program for both undergraduate and graduate students focused on transport and fate of organic pollutants, including a strong community outreach component focused on human exposure to toxic contaminants.

ENVR, TOXI, ANYL

Abstract Title: *Investigating sources, fates, and biological effects of emerging organic contaminants using innovative passive monitoring tools and integrative measures of toxicity*

34. Mohan Qin, Dept. of Civil and Environmental Engineering, Virginia Polytechnic Institute and State University, 406 Durham Hall, Blacksburg, VA 24061. mohanq@vt.edu; Shandong University (B.E., 2010); Peking University (M.S., 2013), Dr. Huazhang Zhao, Synthesis of a novel organic silicate aluminum hybrid coagulant and its coagulation behavior for organic removal; Virginia Tech (Ph.D., anticipated 2017), Dr. Zhen (Jason) He, Resource recovery by osmotic bioelectrochemical systems towards sustainable wastewater treatment. First Place for Wastewater Presentation in Water JAM 2016; 2015 Innovation Award for Best Technological Advancement from International Society for Microbial Electrochemistry and Technology (ISMET); Third Runner-up in the Reclaim Video competition (Title: Reclaiming is to recovery nutrient, energy and water, all in on by microbial electrolysis cell-forward osmosis), (Mar. 2015). <https://sites.google.com/a/vt.edu/mohanqin/>

In research, I seek to advance technology for resource recovery from wastewater and development of wastewater treatment systems. During my Ph.D. study, I focus on the integration of bioelectrochemical systems and forward osmosis to recover water, energy, and nutrients from wastewater. In my future research, I will keep working on the water–energy–food nexus and increase knowledge of the process mechanisms for resource recovery. In addition, I have been a teaching assistant in the environmental and water resources (EWR) seminar course for one year and have already learned three courses for engineering education. I want to teach and direct research at a research university.

ENVR, BIOT

Abstract Title: [*Coupled microbial electrolysis cell-forward osmosis system for sustainable wastewater treatment and resource recovery*](#)

35. Michael J. Shreve, Dept. of Civil and Environmental Engineering, The Pennsylvania State University, 212 Sackett Building, University Park, PA 16802. mjs697@psu.edu, 814-730-0272; The Pennsylvania State University (B.S., honors, 2010; Ph.D., anticipated 2017), Dr. Rachel Brennan (CEE-EnvE), The potential for endogenous and exogenous fungi to enhance the removal of trace organic contaminants during municipal wastewater treatment. National Science Foundation (NSF) Graduate Research Fellowship (2012); Top Graduate of the College of Earth and Mineral Sciences (2010).

I am interested in bioremediation of environmental contamination, with a specific interest in the contribution of fungi to the degradation of trace organic contaminants (TrOCs) in natural and engineered systems. I have experience in conducting solvent extractions and chromatography to quantify TrOCs, performing bioassays to quantify hormone disrupting activity, and various molecular techniques including next-generation sequencing and bioinformatics to characterize microbial communities. I have mentored graduate and undergraduate students conducting research in our group and taught undergraduate-level material in a formal classroom setting. I would primarily like to teach and direct the research of graduate (master's and Ph.D.) students at a four-year university, but feel strongly about having the opportunity to inspire and empower ambitious undergraduates to begin research careers.

ENVR

Abstract Title: [Removal of trace organic contaminants and estrogenic activity in six full-scale integrated fixed-film activated sludge \(IFAS\) wastewater treatment plants](#)

36. Haoran Wei, Dept. of Civil and Environmental Engineering, Virginia Tech, 325 Stanger St., Blacksburg, VA 24060. haoranw@vt.edu; Shandong University (B.S., 2010); Tsinghua University (M.S., 2013), Dr. Shubo Deng, Three biomass-based activated carbons for carbon dioxide capture; Virginia Tech (Ph.D., 2013–present), Dr. Peter J. Vikesland, Surface-enhanced Raman spectroscopy for environmental analysis: Optimization and quantitation. Ellen Gonter Paper Award in the ACS Environmental Chemistry Division, 2017; Graduate Student Award in the ACS Environmental Chemistry Division, 2017; Student Award in Sustainable Nanotechnology Organization (SNO), 2016.

My Ph.D. work focuses on improving the quantitation performance of surface-enhanced Raman spectroscopy (SERS) for environmental analysis. I have developed a universally applicable approach to mitigate the intrinsic heterogeneity of SERS substrates by normalizing SERS signals with Rayleigh scatterings coming from the same “hot spot.” I have also been applying SERS nanoprobes to study the pH inside micrometer-sized aerosol droplets, which is particularly important for haze formation and pathogen transmission. I want to find a faculty position in a research university.

ENVR, ANYL

Abstract Title: [Quantitative SERS enabled by surface plasmon enhanced elastic scattering](#)

37. Jay R. Werber, Dept. of Chemical & Environmental Engineering, 17 Hillhouse Ave., Room #511, New Haven, CT 06511. jay.werber@yale.edu, 484-241-1502; Washington University in St. Louis (B.S., Chem Eng, Minor in Bio, 2009); Yale University (M.S., 2015; M.Phil., 2016; Ph.D., Chem and Envr Eng, anticipated 2018); Prof. Menachem Elimelech, Permeability and selectivity limits of polymeric and biomimetic desalination membranes. NSF Graduate Research Fellow (2013–2017); Abel Wolman Fellow, American Water Works Association (2017–2018); Co-Valedictorian and Co-Student Marshal, Washington Univ. School of Engineering (2009).
<http://elimelechlab.yale.edu/people/jay-werber>

My Ph.D. work has focused on membrane-based separations, particularly for desalination applications. I have gained expertise on the fundamental transport properties of conventional polymeric desalination membranes and biomimetic membranes that would incorporate natural (protein) and synthetic water channels within the membrane selective layer. I aim to become a professor of chemical or environmental engineering, or both, at an R-1 university in the United States. As a professor, I plan to continue research in membrane-based separations, with a major focus on organic solvent separations with the stretch goal of replacing distillation in the petrochemical industry. I also plan to continue research on water treatment, with major efforts on desalination and the development of membranes with special ion selectivity for efficient water treatment and capture or reuse, or both, of heavy metals.

ENVR, ENFL

Abstract Title: [Water-solute permselectivity limits of biomimetic desalination membranes](#)

38. Elena Khlebnikova, Dept. of Chemical Engineering of Fuels and Chemical Cybernetics, Tomsk Polytechnic University, Tomsk, Russia. elena.khle@gmail.com; Tomsk Polytechnic University, Tomsk, Russia (B.S., Processes and Devices of Chem Eng, 2011; M.S., Processes and Devices of Chem Eng, 2013), Dr. Natalia Usheva; Tomsk Polytechnic University (Ph.D., Processes and Devices of Chem Eng, 2013– present), Prof. Elena Ivashkina, Intensification of benzene with ethylene alkylation. Medal, Scientific and Technical Creativity of the Youth Competition, All-Russia Exhibition Center, Moscow, for Achievements in Technical Scientific Work (2012); Diploma, 3rd place, University of Mines, Saint Petersburg, Russia, National Conference–Competition of Graduate Students (2013); Diploma, 2nd place, University of Mines, Saint Petersburg, Working Group, Metallurgy, Physical and Chemical Regularities of Technological Processes at the International Forum–Competition of Young Researchers, Topical Issues of Rational Use of Natural Resources (2013); Bronze Medal and Diploma, Tomsk Polytechnic University, Merit to Tomsk Polytechnic University (2013); Medal, Scientific and Technical Creativity of the Youth Competition, All-Russia Exhibition Center, Moscow, Laureate of All-Russia Exhibition Center (2014).

I'm interested in researching oil and gas processing, oil refining and petrochemical processes. My postgraduate research studied benzene with ethylene alkylation and developed a mathematical model that takes into account the influence of chemical reactions' thermal effects on micro- and macrostructural hydrodynamic phenomena on the kinetics of mass transfer and selectivity of chemical process in a gas–liquid reactor. I developed my skills highly as an assistant and an engineer. In engineering companies, I worked persistently and effectively on personal training, improving, regularly getting new knowledge in oil and gas field design. At Southampton University, UK, I got a great opportunity to work with highly qualified research group and use one of the best academic computational facilities in Europe. I hope to grow professionally further and looking for a Postdoctoral Associate position.

FUEL, COMP

Abstract Title: [*Alkylation of benzene with ethylene in the presence of zeolite catalyst: Mathematical modelling of reactor*](#)

39. Jonathan D. Caranto, Dept. of Chemistry and Chemical Biology, Cornell University, S.T. Olin Lab, Room 678, 162 Sciences Dr., Ithaca, NY 14853. jdc30@cornell.edu; Illinois Institute of Technology (B.S., 2003; B.S., Molecular Biochem and Biophysics, 2003); University of Texas at San Antonio (Ph.D., 2013), Prof. Donald M. Kurtz, Jr., The nitric oxide reductase mechanism of flavo-diiron proteins; Postdoctoral Research Associate at Cornell University (2013–present), Prof. Kyle M. Lancaster, The enzymology of nitrification pathways. Award: NextProf 2015.

<http://linkedin.com/in/jonathan-caranto-63654a31>

I am interested in studying biosynthetic pathways that incorporate NO into natural products that exhibit antibiotic activity. We will use genetic and bioinformatic approaches to discover novel metalloenzyme activities; kinetics and spectroscopy will be used to elucidate the mechanisms of these enzymes. Using this research as a foundation, my future goals are to study allosteric control of metalloenzymes, discover new antibiotic and anticancer agents, and engineer enzymes to aid in synthetic methodologies. I am most interested in teaching undergraduate- or graduate-level biochemistry or inorganic chemistry. I have a strong record in mentoring and working to broaden the participation of underrepresented minorities in science. I want to teach and direct a research lab at a Ph.D.-granting university.

INOR, BIOL

Abstract Title: [Hydroxylamine oxidoreductase activities and bacterial ammonia oxidation pathways](#)

40. Michaela Carlson, 2016 S. Orchard St. Apt. D, Urbana, IL, 61801. mcarlson42@me.com, 520-203-6345; Grinnell College (B.A., 2013); University of Illinois at Urbana–Champaign (Ph.D., anticipated 2018), Prof. Thomas Rauchfuss (Inorg Chem) and Prof. Josh Vura-Weis (Physical Chem), Structural and spectroscopic studies of various [FeFe]- and [NiFe]-hydrogenase model complexes. Buhrk Fellowship State Match (2015–2017); Teaching Excellence Fellowship (2014–2015); Virginia Bartow Scholar (2013–2014); Honors in Chemistry (2013); Luther Erickson Summer Research Fellowship (2012).

I am passionate about teaching and creating an organometallic research group at a small liberal arts college. I am eager to create chemistry courses (such as forensics or the chemistry of food) that would be interesting for students from both non-scientific and scientific backgrounds. While at UIUC, I designed the homework assignments and exams for an upper-level inorganic section. I was also a discussion section leader for general chemistry, where I lectured and led workshop style class assignments. My future research group would focus on the synthesis (using glove box and schlenk line techniques) and characterization of hydrogen fuel catalysts through NMR, cyclic voltammetry, IR and UV-Vis spectroscopy. I hope to inspire my students (both from scientific and non-scientific backgrounds) to become interested in renewable energy sources through my teachings and research.

INOR

Abstract Title: *Diiron complexes with new proton-relay ligand platforms*

41. Jiawei Chen, Dept. of Chemistry, Columbia University, 3000 Broadway, New York, NY 10027. jc4756@columbia.edu; Wuhan University (B.S., 2008); Rutgers University—Newark (Ph.D., 2014), Dr. Frieder Jäkle, Planar chiral Lewis acids and Lewis pairs based on ferrocene; Postdoctoral Researcher at Colorado State University (2014–2016), Dr. Eugene Y.-X. Chen, Highly Lewis acidic organoboranes and organoalanes for small molecule activation and polymer synthesis; Postdoctoral Researcher at Columbia University (2016–present), Dr. Jack Norton, Insertion of isonitriles into Group 4 metal diene complexes.

<https://www.linkedin.com/in/jiawei-chen-84683765/>

https://www.researchgate.net/profile/Jiawei_Chen19

My research lies at the interface between inorganic, organometallic and polymer chemistry. In particular, I aim to develop new Lewis acid/Lewis pair systems for small molecule activation, frustrated Lewis pair (FLP) chemistry, and polymer synthesis. My future interest will focus on: 1) investigating structural features, bonding interactions, and electron accepting properties of new main group Lewis acids; 2) applying acidic catalysts with unexceptional reactivity to small molecule activation and subsequent transformations; 3) identifying suitable Lewis pair combinations for FLP chemistry and polymer synthesis. I have been a TA for general chemistry and advanced synthesis lab. I also have experience on mentoring undergrads and assisting the organization of NSF high school outreach programs. I prefer a tenure-track position in a graduate degree-granting institute.

INOR, CATL, POLY

Abstract Title: [*Planar chiral, redox active and strongly Lewis acidic organoboranes and organoalanes: Isolation, structural characterization and diverse catalysis*](#)

42. Robert J. Comito, Dept. of Chemistry, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA 02139. rcomito@mit.edu, 201-421-7877; Rutgers University (B.A., 2009), Prof. Spencer Knapp, Synthetic medicinal chemistry; Princeton University (Ph.D., 2014), Prof. David MacMillan, Asymmetric catalysis and organic synthesis; Postdoctoral Associate at Massachusetts Institute of Technology (present), Prof. Mircea Dincă, Single-site heterogeneous catalysis in metal-organic frameworks.

My research focuses on selective catalytic methods for small molecule and polymer synthesis. For my Ph.D., I studied chiral amine and transition metal catalyzed carbon–carbon bond formation, developing stereoselective methods for heterocycle and natural product synthesis. Currently, I am studying selective alkene upgrading using metal-organic framework catalysts. Through this effort, I have maintained inter-university collaborations and mentored junior researchers. Along these lines, I have taught both undergraduate organic chemistry and graduate inorganic chemistry. Building upon this experience, I am interested in starting my own laboratory at a Ph.D.-granting institution. My future research interests include small molecule and polymer synthesis using main group catalysis, addressing transformations that are currently challenging by conventional transition metal-catalyzed methods.

INOR, CATAL, POLY, ORGN

Abstract Title: *The secondary building unit as metalloligand: Structural and mechanistic insight into catalysis at metal-organic framework nodes*

43. Honore Djieutedjeu, 600 Rose St., Lexington, KY 40506. djieuteh@umich.edu, honore.djieutedjeu@uky.edu, 734-829-8429; University of Dschang, Cameroon (B.S., 2001); University of Yaoundé I, Cameroon (M.S., plus High Schools' Teacher Grade II Diploma, 2003; plus D.E.A. [Diploma of Advanced Studies], Mat Chem, 2004); University of Michigan (Ph.D., Mat Sci and Eng, 2013), Prof. Pierre Ferdinand Poudeu Poudeu; Lyman T. Johnson Fellow at the University of Kentucky, Lexington 2016–present), Prof. Beth S. Guiton, Undertaking and leading new project on multifunctional heterostructured materials based on the graphene-like system, synthesizing magnetic nanostructured oxides and chalcogenides; Postdoctoral Research Associate at the University of Michigan, Prof. Pierre Ferdinand Poudeu Poudeu, Leading the complex metal chalcogenide projects, in charge of the group's magnetic properties measurement. Lyman T. Johnson Postdoctoral Fellowship, Office of Vice-President for Research, University of Kentucky; Rackham graduate student travel grant for nature frontier of electronic materials conference 2012; Third best junior graduate poster of University of New Orleans, Department of Chemistry annual research presentation, University of New Orleans, LA; Among the 50 graduate students selected for the thirteenth National School of Neutron and X-ray Scattering, Oak Ridge, and Argonne National Laboratory, June 11–25, 2011; Selected to participate the International Summer School on Magnetism, May 21–28, 2011. Reviewer of: *Inorganic Chemistry* (2013–present); *Journal of Electronic Materials* (2013–present); *RSC Advances* (2014–present).

My research has focused specifically on the synthesis, synthesis methodology, fundamental and experimental investigation of bulk solid state materials. Interested in advanced materials for our time energy issues using 2-D transition metal Dichalcogenides and graphene-like materials, my goals are to attract talented future scientists in the field of materials chemistry and motivate them to explore, create, and investigate the nanostructured multifunctional devices for optics, optoelectronic and light emitting diode. I am also interested in developing and creating nanostructure enabling efficient fuel cell and Li-ion battery, development of a cost-effective process for device fabrication and testing. I am interested in teaching and own dynamic materials chemistry and materials science research laboratory in graduate research institution (Ph.D. and M.S.) or 4-year undergraduate institution.

INOR, PHYS, ANYL, FUEL

Abstract Title: [Low temperature growth of ZrSe₂/HfSe₂ thin film and nanostructured complex metal chalcogenide MnSb₂Se₄](#)

44. Sarina J. Dorazio, Georg-August-Universität Göttingen Institut für Anorganische Chemie, Tammannstraße 4, 37077 Göttingen, Deutschland. sarina.dorazio@chemie.uni-goettingen.de; Genesee Community College (A.A., A.S., 2007); The State University of New York at Buffalo (B.A., cum laude, 2008; Ph.D., 2013), Dr. Janet R. Morrow, Transition metal ion paraCEST contrast agents for MRI; Postdoctoral Research Associate at University of Connecticut (2013–2015), Dr. Christian Brückner, Synthesis and characterization of indachlorins; Alexander von Humboldt Postdoctoral Research Fellow at Georg-August-Universität Göttingen Institut für Anorganische Chemie (2016–present), Dr. Franc Meyer, Group 10 metal complexes of an expanded porphyrin. Alexander von Humboldt Postdoctoral Research Fellowship (2016); ACS Division of Inorganic Chemistry Travel Award (2013); Women Chemists Committee/Eli Lilly Travel Award (2012); Mattern-Tyler Teaching Award—UB Chemistry Department (2011); Community College Internship (DOE sponsored)—Pacific Northwest National Lab, WA (2007). Please visit my online profiles at:

<https://www.linkedin.com/in/sjedorazio/>

https://www.researchgate.net/profile/Sarina_Dorazio

I have journeyed from a community college in rural New York to SUNY Buffalo, where I earned my Ph.D., then a first postdoctoral position at UCONN. Having secured support through the Alexander von Humboldt foundation, I continued on as a postdoctoral fellow in Germany. My work spans synthetic porphyrinoid chemistry, paramagnetic macrocyclic complexes, and bimetallic systems. I will mentor students at a research-intensive university in organic synthesis and inorganic chemistry. My group will create molecules for biomedical applications, light harvesting, and information storage. Colorful porphyrinoids are central to these research programs, and they are accessible to undergraduates and secondary school students, providing the foundation for outreach-associated endeavors.

INOR, ORGN

Abstract Title: *[Journey of macrocyclic proportions: From developing transition metal contrast agents to expanding the capabilities of porphyrinoid systems containing non-pyrrolic heterocycles](#)*

45. Gaya R. Elpitiya, Dept. of Chemistry, University of Tennessee, Dabney-Buehler Hall, 1416, Circle Drive, Knoxville, TN 37996-1600. gelpitiy@utk.edu, 803-381-6877; University of Colombo, Sri Lanka (B.S., 2009); University of South Carolina (Ph.D., 2015), Prof. Richard D. Adams, Polynuclear iridium-bismuth cluster complexes: Synthesis, chemistry, and applications towards bi-metallic catalysis. Joseph W. Bouknight Teaching Awards, University of South Carolina (USC) (2012 and 2014); Graduate School Travel Award, USC (2015); JR Durig Travel Award, USC (2015); Oakwood Products Best Poster Award (2015); PFF credential (Preparing for Future Faculty, 2015); Winner of the Women in Science Symposium Poster presentation, USC (2015).

www.linkedin.com/in/gaya-elpitiya

I would like to take my synthesis and characterization experiences in transition metal-main group metal cluster chemistry and N-heterocyclic carbene chemistry to the next level and develop a novel research program based on abnormal carbenes, especially cyclic alkyl amino carbenes, which can be used for both heterogeneous and homogeneous catalysis. I'm interested in teaching general chemistry, advanced inorganic chemistry, X-ray crystallography for undergraduate and graduate students and tailor my research interests according to my student group, whether it is at a PUI, a comprehensive college, or a Ph.D. institution. Students who join my research program will master air-sensitive synthesis techniques including the use of schlenk lines and glove box, Single Crystal X-ray diffraction for structure determination, various other spectroscopic techniques, and computational calculation methods.

INOR, ANYL

Abstract Title: *Unprecedented chromium-ligand multiple bonding and oxidative group transfer reactions supported by a macrocyclic N-heterocyclic tetracarbene*

46. Emil A. Hernandez-Pagan, Dept. of Chemistry, Vanderbilt University, 7330 Stevenson Center, Nashville, TN 37235. emil.a.hernandez@gmail.com; University of Puerto Rico, Mayagüez (B.S., 2005); Pennsylvania State University (Ph.D., 2011), Dr. Thomas Mallouk, Template-assisted electrodeposition of one-dimensional nanostructures for sensing and solar energy applications; Postdoctoral Researcher at Vanderbilt University (2012–2013), Dr. Janet Macdonald, Synthesis of CuInS₂-metal hybrid nanostructures; Amgen (2013–2016), Specialist Quality Complaints; Postdoctoral Researcher at Vanderbilt University (2017–present), Dr. Janet Macdonald, Synthesis of Au₂S via cation exchange of Cu₂S nanoparticles and Nonlinear optical properties of Au-CuS plasmonic nanostructures.

After working for a few years in industry, I realized my true passions are research and teaching. For this reason, I decided to do a second postdoc. My main research interests are (a) control of nanoparticles structure through ligand surface chemistry, (b) nanoparticles structure-(photo)catalytic and magnetic properties correlation, and (c) exploitation of nanoparticles surface ligands for catalytic applications. I want to build my research program and teach at a Ph.D.-granting or regional comprehensive university. I want to be actively engaged in outreach and recruitment of underrepresented minorities.

INOR, NANO

Abstract Title: *Gold (I) sulfide nanostructures obtained via cation exchange of copper sulfides*

47. Matthew J. Jurow, Molecular Foundry, Lawrence Berkeley National Laboratory, One Cyclotron Rd., Mail Stop: 67R6110, Berkeley, CA 94720. mjurow@lbl.gov; 201-452-6308; University of Southern California (B.A., 2007); City University of New York Graduate Center (Ph.D., 2012), Prof. Charles M. Drain, Designed, synthesized, and characterized photoactive materials including organic and organometallic dyes, fullerenes, and hybrid materials designed to assemble into hierarchical nanoscale assemblies, plus collaboration with Brookhaven National Laboratories; Postdoctoral Research at University of Southern California (2013–2015), Prof. Mark E. Thompson, Designed, synthesized, and characterized organometallic phosphors, high-energy organic host materials, and highly efficient OLED devices, plus studied nanoscale orientation and controlled direction of light emission; Postdoctoral Research at Lawrence Berkeley National Laboratory (2016–present), Dr. Yi Liu, Prof. Ting Xu, Prof. A. Paul Alivisatos, Studying the basic synthetic and photophysical properties of inorganic perovskite nanocrystals and collaborating with UC Berkeley to develop hybrid nanoparticle/polymer materials for energy storage. Anton B. Burg Foundation Postdoctoral Fellowship award (2014); DOE Nanoscale Science Engineering and Technology grant for “Organic/inorganic nanocomposite program” (2017); DOE Solid State Lighting grant: “Getting all the light out: Eliminating plasmon losses in high efficiency white organic light emitting devices for lighting applications” (\$1,747,638; 2015); NSF CBET SusChEM grant: “Materials and architectures for high efficiency organic photovoltaics” (\$300,000; 2015).

I am primarily interested in creating new photoactive materials with customizable nanoscale architectures to control the absorption and emission of light, charge transport, and energy storage properties. I have an interdisciplinary and collaborative background designing, developing, and characterizing organic, inorganic, and hybrid materials using a range of spectroscopies, synchrotron techniques, and electron microscopy. The broader impacts of my research in energy technologies, coupled with the interdisciplinary nature of my work, will appeal to students and funding agencies alike. I have prepared and delivered both lecture and laboratory courses and worked at an extremely diverse set of institutions. I would like to teach and direct research at an exceptional, undergraduate-focused four-year college with bright and motivated students or a large and diverse research university.

PHYS, INOR, COLL

Abstract Title: [Nanoscale optimization of materials for optoelectronics](#)

48. A. Nano

Abstract Title: [Rhodium-cyanine fluorescent probes for detection and signaling of mismatches in DNA](#)

49. Sameer Patwardhan, Argonne-Northwestern Solar Energy Research Center, Northwestern University, 2145 Sheridan Rd., Evanston, IL 60208. sameerpatwardhan@gmail.com; Indian Institute of Technology Bombay, India (M.S., 2007); Delft University of Technology, The Netherlands (Ph.D., 2011), Dr. Laurens Siebbeles and Dr Ferdinand Grozema, Charge carriers and excited states in supramolecular materials; Postdoctoral Scholar at Northwestern University (2012–present), Dr. George Schatz, Nanostructured materials for photovoltaic and electrochemical energy conversion.
sites.northwestern.edu/spatwardhan

I am a materials chemist interested in computational design, synthesis, and characterization of nanostructured materials, and its use in photovoltaic and electrochemical device applications. In particular, I am interested in atomistic structure and optoelectronic properties of hybrid materials and interfaces involving perovskites, metal-organic frameworks, and metal-oxides. Over the past three years, I have translated proprietary Northwestern technologies for undergraduate education, and I have implemented new experiments in the undergraduate curriculum at Northwestern and beyond. I will continue to bring relevant science into classrooms while motivating undergraduates to participate in research projects in my group.

ENFL, PHYS, CHED

Abstract Title: [Nanomaterial synthesis using atomic layer deposition](#)

50. Jade K. Pratt, Dept. of Chemistry, University of California, Davis, One Shields Ave., Davis, California 95824. jkpratt@ucdavis.edu; Ithaca College (B.S., 2011); University of California, Davis (Ph.D., 2017), Professor Philip Power (Inorg Chem), Synthesis and characterization of transition metal thiolate complexes.

I am interested in the synthesis of unusual low valent inorganic complexes that will be characterized by NMR, IR, UV-Vis and X-ray crystallographic techniques. I have engaged diverse student populations through the teaching of general, organic, and inorganic chemistry courses. I have teaching experience as both a head teaching assistant at a research-focused university and as an adjunct faculty member at the community college level. I want to educate and mentor undergraduate students through both classes and research at a primarily undergraduate institution.

INOR

Abstract Title: [Synthesis and characterization of homoleptic copper \(I\) thiolate complexes](#)

51. J. Scepaniak

Abstract Title: *Those who wander are not lost, a two-continent academic journey: Molecular transformations by first-row transition metals, late transition metal organometallics, teaching, and establishing an independent research presence in contrast agents for MRI*

52. Yi Shen, Dept. of Chemical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Ave., Rm 66-503, Cambridge, MA 02139. yishen@mit.edu; Nanjing University, China (B.S., 2010), Dr. Weiping Ding, Selective oxidation of toluene on oxide nanoparticle catalysts; University of South Carolina, Columbia (Ph.D., 2015), Dr. Andrew Greytak, Quantum dot metrics for preparative chemistry and fluorescence applications; Postdoctoral Associate at MIT, Dr. Klavs Jensen, Continuous flow platform for studying synthesis, purification and surface modification of quantum dots.

My research interest is the surface chemistry and surface modification of nanomaterials. During my Ph.D. study, I designed a novel nanocrystal purification technique and performed sequential chemistry on the well-characterized nanocrystals to study their photo-physical properties or to apply for biological imaging. My postdoc research emphasizes using a flow chemistry platform to study the synthesis, purification, and surface modification of quantum dots in the continuous system. I worked as a teaching assistant for five different courses at graduate school and was awarded teaching awards twice. I also participated in a certified teaching program and mentored two students on their master theses at MIT. I would like to teach and direct research at a doctoral degree-granting university or a regional comprehensive and four-year undergraduate university.

INOR, COLL

Abstract Title: *Sequential chemistry study of well-isolated and characterized quantum dots using batch and continuous flow platforms*

53. Paul F. Smith, Dept. of Chemistry, Stony Brook University, Stony Brook NY 11794.
Paul.f.smith@stonybrook.edu; 609-257-8121; Gettysburg College (B.S., Chem and Math, 2010); Rutgers University (Ph.D., Inor Chem, 2015), G. Charles Dismukes, Study of the mechanisms and active sites of homogeneous and heterogeneous cobalt and manganese water oxidation catalysts; Postdoctoral Researcher at Stony Brook University and Brookhaven National Lab (2016–present), Esther Takeuchi, Kenneth Takeuchi, and Amy Marschilok, Electrochemistry of materials in battery systems: Iron and manganese oxides. NSF IGERT Renewable and Sustainable Fuels Graduate Fellowship; NSF East Asia-Pacific Summer Institute 2011 Fellowship, Rutgers Reid Award (Highest Honors), Gettysburg J. Rogers Musselman Award.
www.linkedin.com/in/paul-smith-09265768
www.researchgate.net/profile/paul_smith

Kindly consider my interest in positions offered at four-year colleges or comprehensive universities. Since 2007, I have served in some capacity as a tutor, in-lab mentor, or teaching assistant. I can cite experience giving presentations on three continents, as well as recent efforts in designing graduate coursework alongside a SUNY distinguished teaching professor. To date, 90% of undergraduate students have rated my teaching effectiveness above average or excellent. I am motivated to improve this number going forward. Further, I can propose a number of research programs catered to be flexible to infrastructure. My research experience has focused on electrochemical studies of complex crystalline oxides; however, a concurrent goal is to prepare simpler, molecular compounds that are structurally similar and may mimic functional properties.

ENFL, INOR, CATL

Abstract Title: [Molecular to mesoscale: Identifying atomic-level structural features of nanocrystalline manganese oxides critical to understanding electrochemistry](#)

54. Edmund Chun Ming Tse, 51 Grace Terr., Pasadena, CA 91105. etse@caltech.edu, 858-210-1025; The University of Virginia (B.S., Chem, Materials Sci specialty, 2011), T. B. Gunnoe, Transition metal complexes for methane C-H bond activation and olefin hydroarylation; The University of Illinois at Urbana–Champaign (Ph.D., Inor Chem, 2016), A. A. Gewirth and T. B. Rauchfuss, Facilitating, understanding, and controlling the oxygen reduction reaction for fuel cell technology using (1) laccase-inspired tricopper molecular catalysts, (2) a high temperature and pressure reaction vessel, and (3) a hybrid bilayer membrane electrochemical platform; Postdoctoral Fellow (Div of Chem and Chem Eng) at The California Institute of Technology (2016–present), J. K. Barton, DNA damage recognition enabled by repair proteins containing redox-active [4Fe4S] metallocofactors. Croucher Foundation Fellowship for Postdoctoral Research (2016–2018); Poster Award at the ICCAI conference (2016); Theron Standish Piper Award for outstanding research, dissertation, and thesis in inorganic chemistry (2015); Eastman Travel Grant to attend a Gordon Research Conference (2014); Croucher Foundation Scholarship for Ph.D. studies (2013–2014).

<http://scholars.croucher.org.hk/scholars/tse-chun-ming-edmund>

My interests are broad, but they are centered around catalysis, self-assembly, and biological systems. My proposed work includes developing bioinspired multi-metal electrocatalysts for proton-coupled electron transfer reactions central to renewable and biological energy conversion schemes. My group will feature students interested in chemical synthesis, biophysical modeling, surface functionalization, and device fabrication. I taught an advanced instrumental analysis course and a graduate-level electrochemistry course. I was recognized as one of the best teaching assistants when I taught a general chemistry lab class at the University of Illinois at Urbana–Champaign. I also obtained a certificate of interest in university-level teaching at the California Institute of Technology. I would like to guide and motivate students and postdocs at an R1 or R2 institution.

INOR, ANYL, PHYS, ENFL, CATL, BIOL, COLL

Abstract Title: *DNA damage recognition mediated by repair proteins carrying [4Fe4S] clusters and understanding proton-coupled electron transfer processes using a lipid-modified electrochemical platform*

55. Wen Zhou, Dept. of Chemistry, Massachusetts Institute of Technology, 77 Massachusetts Ave., 18-425, Cambridge, MA 02155. wzhou@mit.edu; Jilin University (B.S., Applied Chem, 2006); Brandeis University (Ph.D., Inorg Chem, 2013), Prof. Christine M. Thomas, Synthesis and catalytic application of heterobimetallic complexes; Postdoctoral Researcher at Washington University (2013–2016), Prof. Liviu M. Mirica, High-valent organometallic nickel and palladium complexes mediated chemical transformations (NSF); Postdoctoral Associate at Massachusetts Institute of Technology (2016–present), Prof. Stephen J. Lippard, Platinum based anticancer drug design and activity study (NIH).

I am looking for a faculty position in a research university or institute. I am interested in the synthesis of transition metal complexes, with the ultimate goal of discovering new metal-based anticancer drugs and uncovering new approaches to the activation and functionalization of small molecules such as CH₄ and N₂. Although I am proposing two research projects, the underlying theme in my research program is synthetic inorganic and organometallic chemistry, which enables the understanding of the roles of metal ions in biological processes and organic transformations. My research plan involves a number of fundamental aspects of inorganic, organic, biological, and organometallic chemistry and should provide students with a means of learning a wide range of new concepts and techniques.

INOR, ORGN

Abstract Title: [*High-valent organometallic nickel complexes mediated C-H bond activation and bond formation reactions*](#)

56. Salvador B. Muñoz III, Dept. of Chemistry, University of Rochester, 120 Trustee Rd., Rochester, NY 14627. smunoz4@ur.rochester.edu; University of Texas at El Paso (B.S., 2008); New Mexico State University (Ph.D., 2015), Dr. Jeremy M. Smith, Synthesis and spectroscopic investigation of new tris(carbene)borate ligands: Efforts toward new iron(IV)nitrides. Ruth L. Kirschstein National Research Service Award Postdoctoral Fellow (2015–present), Dr. Michael L. Neidig, Isolation and characterization of catalytically relevant species in C–C cross-coupling mediated by simple iron salts and alkyl Grignards.

My research interests will focus on the preparation and characterization of novel transition-metal complexes geared toward small molecule activation. One major objective will be to harness super electron donor ligands to engender earth-abundant metals, such as iron, with multi-electron reactivity. To this same end the preparation of new multimetallic coordination complexes is also of interest. Polymetallic complexes, composed of elements which commonly participate in single electron processes as single metal centers, can function in concert as reservoirs of electrons for small-molecule activation. Within my postgraduate career I have been fortunate enough to mentor various undergraduate students as well as incoming graduate students, a truly rewarding experience. I look forward to continuing to mentor budding young scientists as we seek to expand our understanding of the molecular world.

INOR

Abstract Title: *From high valent Iron nitrides to catalytically relevant low valent homoleptic iron alkyl complexes*

57. Jae-Ho (Jay) Lee, Nuclear Medicine Dept., Clinical Center, National Institutes of Health, Bldg. 21/RM 136, Bethesda, Maryland 20892. leejaeho@mail.nih.gov; Seoul National University (B. S.; M.S. Chem. Tech., 1994), M.S., Dr. Jihwa Lee, A study on the improvement of flame retardancy of HDPE by plasma treatment; University of Maryland (Ph.D., Chem. Eng., 2006), Dr. Srinivasa R. Raghavan, Soft materials based on vesicle and biopolymers; Postdoctoral Fellow at Clinical Center, NIH (2006–2008), Dr. Joseph A. Frank, Multimodal MRI contrast agents for stem cell labeling; Postdoctoral Fellow at NCI, NIH (2008–2010), Dr. Robert Blumenthal, Liposomal drug delivery; Scientist at NMD, CC, NIH (2010–present), Dr. Chang H. Paik, Cancer immunotherapy.

I am interested in nanomedicine, cancer therapy, and computer models. I hope to help students to learn these areas. I assisted in chemical engineering courses and mentored students. I want to teach and direct the research of undergraduate (and graduate) students at a four-year college or research-oriented university.

MEDI, COLL

Abstract Title: *Cancer immunotherapy, cell imaging and drug delivery from self-assembled structure*

58. Kelly A. Teske, University of Connecticut, Pharmaceutical Science Dept., 69 N. Eagleville Rd., Unit 3092, Storrs, CT 06269-3092. kelly.teske@gmail.com, 860-486-8377, cell: 815-222-9301; Illinois State University, Normal, IL (B.S., Chem; B.S. Biochem and Molecular Bio, 2010); University of Wisconsin–Milwaukee, WI (Ph.D., Org (Medicinal) Chem, 2015), Prof. Alexander (Leggy) Arnold, Part I: The development of non-secosteroidal vitamin D receptor modulators, Part II: The development of a universal GTPase assay; Postdoctoral Researcher in Medicinal Chemistry at University of Connecticut–Storrs (2015–present), Prof. M. Kyle Hadden, (1) Development of azole antifungal analogues for the treatment of hedgehog dependent cancers, (2) Targeting methyllysine binding domains, specifically the ADD domain of the chromatin remodeler ATRX, to investigate its epigenetic role in cancers such as pediatric glioma and glioblastoma. Dr. and Mrs. George Sosnovsky Award for Excellence in Graduate Research, University of Wisconsin–Milwaukee (2015); ACS MEDI-Chem Travel Award (2014); University of Wisconsin–Milwaukee Research Poster Award (2014); The Gloria Moczynski Student Teacher Award, University of Wisconsin–Milwaukee (2013); The American Chemical Society Undergraduate Award in Inorganic Chemistry, Nominated by Illinois State University Dept. of Chemistry and Biochemistry (2010).

<https://www.linkedin.com/in/kelly-teske-751095aa>

<http://hadden.lab.uconn.edu/>

I am interested in teaching in a chemistry or medicinal chemistry department of a comprehensive university, which will allow me to focus more on education while also maintaining a research lab. The research I aim to conduct will be interdisciplinary, using organic synthesis and biochemical techniques to answer medicinal questions. I have primarily focused my career on cancer research and will likely continue that for my own research lab. I have many years of experience teaching a diverse range of courses as a teaching assistant at the University of Wisconsin–Milwaukee and have also had the opportunity to guest lecture a pharmacy course at the University of Connecticut. I am most interested in teaching organic chemistry courses (undergraduate and graduate levels), but am confident in my ability to teach biochemistry, medicinal/pharmacology and general chemistry courses, as well.

MEDI

Abstract Title: [*Development of azole antifungal analogues to treat Hedgehog dependent cancers*](#)

59. Rene Fuanta, Dept. of Chemistry and Biochemistry, Auburn University, 179 Chemistry Building, Auburn, AL, 36849. rfn0001@auburn.edu; University of Buea, Cameroon (B.S., Microbio, 2010; Masters Courses only, Microbio, 2013); Auburn University (Ph.D., Biochem, anticipated 2018), Dr. Douglas Goodwin (Biochem) and Dr. Angela Calderon (Drug discovery), Towards a high throughput drug screening approach for tuberculosis shikimate kinase, intrinsic protein fluorescence. Cellular and Molecular Biology (CMB) research fellowship, Auburn University (2017); Presidential Excellence Grants (O-S), University of Buea, for outstanding performance, four years consecutively (2010–2014).

http://www.auburn.edu/~goodwdc/Rene_Fuanta.html

<https://www.linkedin.com/in/rene-fuanta-922b276b/>

I am interested in drug discovery and screening at the cellular or subcellular level and mechanistic evaluation of proteins and inhibitors via mass spectrometry, fluorimetry, and other biochemical and microbiological techniques. I want to make a contribution towards the fight against drug resistance and improve understanding of disease pathology, be it in an academic or industrial setting. I have experience in experimental design and analysis, drug screening and inhibition, mechanistic enzymology, mass spectrometry, fluorimetry, etc.

BIOL, MEDI

Abstract Title: *Imparting intrinsic fluorescence as an approach towards rapid inhibitor screening and mechanistic evaluation of tuberculosis shikimate kinase*

60. Andrew H. Aeby, Dept. of Chemistry and Biochemistry, Oberlin College, 119 Woodlawn St., Oberlin, OH 44074. aaeby@oberlin.edu; St. John's University, Minnesota (B.A., 2010); Montana State University (Ph.D., 2015), Dr. Trevor J. Rainey, The examination of chiral X-type ligands in Pd(II)-catalyzed enantioselective oxidative transformations; Postdoctoral Research Fellow at Oberlin College (2016–present), Dr. Jason M. Belitsky, Synthetic methodology towards the creation of eumelanin oligomers.

I am interested in reaction methodology with a focus on hypervalent iodine. I have been the instructor of record for two organic chemistry courses (nonmajors and honors) and will be teaching general chemistry and chemistry of the environment (nonmajors) during the spring semester of 2018. I have assisted in the implementation of a course-based research experience in the bioorganic chemistry lab class and have mentored multiple students (both undergraduate and graduate) in the research lab. I was a teaching assistant for seven different classes (more than 30 sections) and am currently the coordinator of Socializing with Scientists, an informal weekly gathering of students, faculty, and staff to discuss science topics. I would like to teach and direct independent research at a primarily undergraduate, liberal arts institution.

ORGN

Abstract Title: *Towards a modular approach to Eumelanin oligomer synthesis*

61. Mary Beth Daub, Dept. of Chemistry, University of Wisconsin–Madison, 1101 University Ave., Madison, WI 53706. mdaub@wisc.edu; Williams College (B.A., 2011), Prof. Thomas E. Smith, Toward the asymmetric total synthesis of jerangolid D; University of California, Irvine (Ph.D., 2016); Prof. Chris Vanderwal, A unified synthetic approach toward the kalihinanes; NIH-NRSA Postdoctoral Research Fellow at University of Wisconsin–Madison (2016–present), Professor Tehshik Yoon, Studying the effect of Lewis acids on the triplet energy of Lewis basic substrates.

My research interests are focused on the synthesis of biologically active complex natural products and the development of new photochemical methodologies. In addition to the various positions as a teaching assistant I held during my graduate studies, I gained experience lecturing for an intermediate organic chemistry class that I co-instructed with my adviser, Professor Chris Vanderwal. I have also mentored two undergraduate researchers on independent projects during graduate school and my postdoctoral fellowship. In my independent career, I plan to build a research program for undergraduate students centered on the development and application of new photochemical methods to natural product synthesis. I would like to pursue a career teaching undergraduate students at a four-year college.

ORGN

Abstract Title: [Exploring the scope of Lewis acid-catalyzed triplet energy transfer: \[2+2\] photocycloaddition and beyond](#)

62. Mary Kathryn Doud, 1 John Carroll Blvd., University Heights, OH 44118. katiedoud@gmail.com, 617-512-3743; Amherst College (B.A., 2000); University of California, Los Angeles (M.S., 2003), Dr. Yves Rubin, Synthesis of open fullerenes; Visiting Assistant Professor at John Carroll University (appointed 2015); Case Western Reserve University (Ph.D., anticipated 2018), Dr. Gregory Tochtrop, Toward an inhibitor for fatty acid binding protein 5, NIH F31 recipient.

The unifying theme of my research focuses on using biophysical methods to better understand protein–small molecule interactions. The goal of this work is to develop chemical probes that can be used to better understand disease with an eye toward realizing potential therapeutics.

BIOL, MEDI, ORGN

Abstract Title: [Design, synthesis, and evaluation of N-phosphonacetyl-L-aspartate derivatives as putative human ATCase inhibitors](#)

63. Justin Foy, Bard College, 30 Campus Rd., Annandale-on-Hudson, NY 12504.
jfoy@bard.edu, 845-752-2311; Saint Michael's College, Colchester, VT (B.S., Biochem, 2008); Dartmouth College, Hanover, NH (Ph.D., 2014), Ivan Aprahamian, Synthesis of aryl-based cyclopentadienyl lithium compounds for self-assembly and proton relays in hydrazone-based rotary switches; Postdoctoral Researcher at Institut Charles Sadron, Strasbourg, France (2014–2016), Integration of molecular switches and machines into polymer materials for mechanically activated gels.

Justin's primary research expertise has centered on synthetic organic chemistry and the design of multi-component molecular switch systems. He pursued his interests in applying their motion on the macroscopic scale by integrating molecular switches and motors into polymeric materials during his postdoc in Strasbourg, France. In the fall of 2016, Justin made the move back to the States to join the Chemistry Department at Bard College as Visiting Assistant Professor. At Bard, he has taught general chemistry lecture and lab courses over the first year of his appointment. His research group at Bard will be investigating the synthesis and properties of new stimuli-responsive materials. In the future, Justin seeks to teach at primarily undergraduate institutions and those that provide a good balance between teaching and research opportunity.

ORGN

Abstract Title: [*Dual-light control of nanomachines that integrate motor and modulator subunits*](#)

64. Sarut Jianrattanasawat, Dept. of Chemistry, Western Michigan University (WMU), 1903 W. Michigan Ave., Kalamazoo, MI, 49008-5413. sarut.jianrattanasawat@wmich.edu, 269-615-2012; Western Michigan University (B.S., 2012), Dr. Gellert Mezei, Layered inorganic-organic networks of pyrazole-4-sulfonate metal complexes and their use in copper anticorrosion protective films; Western Michigan University (Ph.D., anticipated Dec 2017), Dr. Elke Schoffers, Synthesis and characterization of functionalized heterocyclic compounds (e.g., 1,10-phenanthrolines, oxazoles).

<https://sites.google.com/wmich.edu/jianrattanasawat2017>

My research focus is to develop organic material using multifunctional catalytic systems, where various parts are working together to contribute to the overall reaction. My teaching experiences include being a teaching assistant in general chemistry and organic chemistry and a chemistry instructor for the Louis-Stokes Alliances for Minority Participation, as well as mentoring five undergraduate students in the research lab of my supervisor. Also, I have completed a Graduate Student Teaching Intensive course at WMU, a one-year program with an emphasis on pedagogy. I am interested in teaching chemistry at the collegiate level and in conducting research at all levels.

ORGN, INOR

Abstract Title: *Synthesis and characterization of functionalized heterocyclic compounds: 1,10-phenanthrolines and oxazoles*

66. Jacobs H. Jordan, Dept. of Chemistry, Tulane University, 2015 Percival Stern Hall, 6400 Freret St., New Orleans, LA 70118. jjordan2@tulane.edu; University of New Orleans (B.S., Bio, 2009; B.S., Chem, 2010); Tulane University (Ph.D., anticipated 2017), Dr. Bruce C. Gibb, Towards an understanding of the hydrophobic and Hofmeister effects utilizing synthetic hosts. Graduate Honor Board, School of Science & Engineering, Tulane University (2014–present); Southwest Regional Student Presenter Travel Scholarship, 72nd SWRM, Galveston, TX (2016); Division of Organic Chemistry Travel Award, 252nd ACS National Meeting, Philadelphia, PA (2016); 13th International Conference on Calixarenes Travel Grant, Giardini Naxos, Italy (2015); Louisiana Local Section ACS Travel Award, 69th SWRM, Waco, TX (2013).

<https://www.linkedin.com/in/jacobs-jordan-2168a070/>

https://www.researchgate.net/profile/Jacobs_Jordan

I am a physical organic/supramolecular chemist interested in the fundamental interactions that occur at surfaces between molecules in aqueous systems, particularly how dissolved solutes can ultimately affect their binding and assembly properties. I propose to develop novel systems to study these interactions by incorporating synthetic organic techniques and physical organic chemistry utilizing UV-Vis and fluorescent spectroscopy, as well as NMR, ITC, MALDI, ESI, or DLS for characterization. I hope to engage students, especially undergraduates, in this research toward applications and the development of novel sensor systems. I have experience teaching general and organic chemistry laboratories and have assisted with and guest-lectured for organic chemistry courses. I ultimately want to teach undergraduate and graduate students at a regional comprehensive or Ph.D.-granting university.

ORGN, PHYS

Abstract Title: [Water-soluble cavitands: Applications in anion recognition and protein inhibition](#)

67. Hongkun Lin, Dept. of Chemical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA 02139. hklin@mit.edu, hklin@brandeis.edu; Nanjing University (B.S., 2008); Brandeis University (M.S., 2009; Ph.D., 2015), Dr. Isaac Krauss, Synthesis of the skeleton of bromophycolide A and D, Asymmetric homocrotylboration of aldehydes; Research Associate at Massachusetts Institute of Technology (2014–present), Dr. Klavs Jensen, Continuous flow synthesis. Outstanding Teaching Fellow Award, Brandeis University, 2008–2009.

I am interested in organic methodology development and the application flow chemistry to improve reaction efficiency. I assisted in organic laboratory courses during graduate school. I would like to perform independent research in a university or college, and I would like to teach courses of organic chemistry and stimulate students' interests with exciting discoveries in organic chemistry.

ORGN

Abstract Title: *Synthesis of skeleton of bromophycolide A and D asymmetric homocrotylation of aldehydes rapid total synthesis of ciprofloxacin hydrochloride in continuous flow*

67. O. Maduka Ogba, Robbins Postdoctoral Fellow, Dept. of Chemistry, Pomona College, 645 North College Ave., Claremont, CA 91711. o.ogba@pomona.edu; Trinity University (B.S., Computer Sci; minor, Chem, 2011), Prof. Mark Lewis (Computer Sci) and Prof. Steven Bachrach (Chem), Applying the diversity map, a visualization technique, to the protein data bank; Oregon State University (Ph.D., 2016), Prof. Paul Ha-Yeon Cheong, Towards the routine computational investigation of complex organocatalysis and reaction processes; Robbins Postdoctoral Fellowship at Pomona College (2016–2018), Prof. Daniel J. O’Leary, (i) Computational and experimental investigation of molecules containing monodeuterated methyl groups that exhibit long-lived states accessed *via* small proton chemical shift differences, (ii) Automating isotope effects analyses and visualization, (iii) Computational and experimental investigation of the solution behavior of disiloxane diols.

I am a physical organic chemist, trained in computational chemistry and cheminformatics. I seek a tenure-track faculty position at a primarily undergraduate institution, where maintaining active research *and* dynamic teaching and service geared toward a superior and balanced undergraduate education is of high value. Research: My research interest focuses on the fundamental understanding of enzyme active site conformations and on the stereoelectronic factors governing these conformations. My approach is rooted in computational chemistry, spectroscopy, and informatics. Teaching: I have two years of experience teaching general chemistry (lecture and lab), one year with organic chemistry (lecture and lab), and have designed and taught three iterations of a Cheminformatics/Computer Programming for Chemists course at the graduate and undergraduate levels.

COMP, ORGN

Abstract Title: [*Toward the origin of small chemical shift differences in diastereotopic X-CH₂D groups*](#)

68. Tharushi A. Perera, Dept. of Chemistry, Texas State University, 601, University Dr., San Marcos, TX 78666. tap91@txstate.edu, 512-489-3972; Chartered Institute of Marketing (CIM), United Kingdom, (Professional Postgrad, Marketing, 2006); Institute of Chemistry, Ceylon, Colombo, Sri Lanka (Graduateship in Chemistry, 2009); University of Missouri, Columbia (Ph.D., Inor Chem, 2015), Prof. Paul R. Sharp, Chlorine and singlet oxygen photoelimination from organoplatinum(IV) complexes; Postdoctoral Research Associate at Texas State University (2015–present), Prof. Todd W. Hudnall, Design, synthesis, characterization and reactivity of novel carbene-stabilized antimony and bismuth complexes as catalysts for solar energy storage systems.

I received a Ph.D. degree in inorganic chemistry from the University of Missouri–Columbia in July 2015 under the guidance of Prof. Paul R. Sharp. My graduate research was centered around synthetic organometallic chemistry, where I studied the basic mechanisms of energy conversion in chemistry. My postdoctoral research is focused on discovering inexpensive light-absorbing inorganic catalysts—made from earth abundant elements—to replace precious metal catalysts without reducing efficiency for solar fuels production. I have an extensive academic background in chemistry with more than eight years' experience in teaching mainly general, organic, and inorganic chemistry courses. My interest in teaching and carrying out research at a primarily undergraduate institution stems not just from my commitment to quality science education, but also from my desire to enrich the lives of my students.

ORGN

Abstract Title: *Unprecedented reversible Buchner ring expansions by photochemically accessible triplet reactivity from a singlet DAC*

69. Rachelle Quach, School of Chemical Sciences, The University of Auckland, NZ. rachellequach@gmail.com, +64212153255; The University of Auckland (B.S., Med Chem, 2011; B.S., Hons in Med Chem, 2012), Prof. Margaret Brimble, Asymmetric gold-catalysed synthesis of the paecilospirone spiroacetal; The University of Auckland (Ph.D., anticipated 2017), Prof. Margaret Brimble and Dr. Daniel Furtak, Total synthesis of citreoviranol.

I am an organic chemist with a peer-reviewed publication record and five years' laboratory research experience in total synthesis, methodology using asymmetric gold catalysis, and the design of photoreactive biotinylated peptide ligands for target identification. I have assisted in undergraduate organic and medicinal chemistry laboratory courses and would be interested in teaching undergraduate students.

ORGN

Abstract Title: *Total synthesis of citreoviranol*

70. Julia A. Schneider, California NanoSystems Institute, 3229 Elings Hall, University of California Santa Barbara. jschneider@mrl.ucsb.edu; Southern Connecticut State University (B.S., summa cum laude, 2008); McGill University (Ph.D., 2016), Dr. D. F. Perepichka, Tailoring the properties of organic semiconductors through heteroatoms; Postdoctoral Researcher at University of California Santa Barbara (2016–present), Dr. Fred Wudl and Dr. Javier Read de Alaniz, Synthesis of non-fullerene acceptors and n-transport materials for organic photovoltaics. Vanier Canada Graduate Scholar.

I am seeking a tenure-track position at a research-intensive primarily undergraduate institution (PUI). My research is in organic electronics, namely the synthesis and characterization of electronically active polymers and small molecules. A majority of my work is the application-driven organic synthesis of materials, which accompanies computational modeling, optoelectronic characterization, and device fabrication. Device applications include solar cells and transistors. My goal is to introduce talented undergraduate students to organic electronics and polymer/material chemistry as a whole. I hope to broaden my students' notions about what chemistry can accomplish. I am excited to teach organic chemistry, general chemistry, and polymer chemistry. I am also interested in scientific communication and history of chemistry courses.

ORGN, PHYS, POLY

Abstract Title: *Introducing undergraduate researchers to organic electronics*

71. Sami E. Varjosaari, Dept. of Chemistry and Biochemistry, Northern Illinois University, LaTourette Hall, 200 Normal Rd., DeKalb, IL, 60115; svarjosaari@niu.edu, 815-508-9234; University of Oxford (MChem., 2011), Dr. Stephen P. Fletcher, Tandem reactions and asymmetric halogenation; Reservi Upseeri Koulu, Finland (Officer, anti-CBRN, 2012); Northern Illinois University (Ph.D., anticipated May 2018), Dr. Marc J. Adler and Dr. Thomas M. Gilbert, Development of new synthetic methodologies for non-chiral and chiral reductions using hypervalent silicon. Kevin Cull Memorial Teaching Award (2017).

I intend to develop a highly productive research group, ideally at (but not limited to) a Ph.D.-granting university, involving a healthy mix of graduate and undergraduate students. My research interests are in organic synthesis using organoboron and organosilicon compounds, and my initial research goals include developing new synthetic methodologies for metal-free asymmetric halogenations and asymmetric Michael additions. I would also look to collaborate with other faculty members in the department (or other institutions) to broaden the scope and utility of my research and allow students to get a more interdisciplinary experience. I enjoy teaching organic chemistry to majors and nonmajors alike. I helped found the Student Advisory Safety Committee at NIU with the intention to improve the overall safety culture, and I would do so again at any institution I am a part of.

ORGN

Abstract Title: *1-Hydrosilatrane: A chiral Lewis base activated reducing agent for the asymmetric reduction of prochiral ketones to alcohols*

72. Juan M. Artes Vivancos, Lawrence Berkeley National Lab, b75 Hildebrand Hall, UC Berkeley, Berkeley, CA 94720. Jma2@lbl.gov, j.m.artesvivancos@vu.nl; UAB (Autonomous University of Barcelona, B.S., 2007); UB (University of Barcelona, M.S., 2009; Ph.D., 2012), Prof. Pau Gorostiza (Bioengineering) and Prof. Fausto Sanz (Physical Chem), Electrochemical scanning tunneling microscopy and spectroscopy of the redox protein azurin; Human Frontiers Science Program Long-Term Fellowship (2015, declined), Prof. R. van Grondelle, Quantum coherence in photosynthesis: Towards single-molecule light-conversion devices; Marie Skłodowska-Curie Individual Fellowship from Horizon 2020 program European Research Council (2015–present), Prof. R. van Grondelle, Ultrafast spectroscopies for the investigation of quantum coherence in photosynthesis; Visiting Scholar at UC Berkeley, Lawrence Berkeley National Lab (present) and Marie Curie Postdoctoral Fellow at VU Amsterdam; Ph.D. Extraordinary award from the University of Barcelona (2014); Cum Laude (maximum qualification for the Ph.D.).

https://scholar.google.com/citations?user=3kr_xngAAAAJ

https://www.researchgate.net/profile/Juan_Artes

I am interested in doing multidisciplinary, cutting-edge research in physical chemistry and biochemistry. Particularly, I want to apply my experience in single-molecule experiments and nanotechnology (SPMs, electrochemistry, and ultrafast laser systems) to biological and chemical systems and understand ultrafast processes using new techniques. I have 17 publications and more than 320 citations, and I hope to build my own research group in a research-intensive institution. I have been training and guiding M.S. and Ph.D. students, and I want to supervise, train, and direct Ph.D. and M.S. candidates in their projects. I also look forward gaining teaching experience by imparting knowledge through biology and chemistry courses at all levels.

PHYS, BIOL, ANYL

Abstract Title: *Vibrational modes involved in the function of the major light-harvesting complex of higher plants investigated by femtosecond-stimulated Raman spectroscopy*

73. Mikael P. Backlund, Harvard-Smithsonian Center for Astrophysics, 60 Garden St., Cambridge, MA 02138; Department of Physics, Harvard University, 17 Oxford St., Cambridge, MA 02138. mikael.backlund@cfa.harvard.edu; University of California, Berkeley (B.S., Chem, Highest Honors; minor in Math, 2010); Stanford University (Ph.D., Chem, concentration in Chem Physics, 2015), Prof. W. E. Moerner, Development of novel techniques in single-molecule fluorescence microscopy, with applications to super-resolution imaging and particle tracking in cells. Postdoctoral Fellow at Harvard-Smithsonian Center for Astrophysics and Department of Physics, Harvard University (2016–present), Dr. Ronald Walsworth, Novel techniques in optically-detected magnetic resonance microscopy using nitrogen-vacancy centers in diamond. 67th Lindau Nobel Laureate Meeting (2017); Robert and Marvel Kirby Stanford Graduate Fellowship (2010–2013); Erich O. and Elly M. Saegebarth Prize for outstanding undergraduate research (2010).

<https://scholar.google.com/citations?user=kSuuj6UAAA AJ&hl=en>

My lab will develop and apply new methods for nanoscale optical and magnetic imaging. I seek clever solutions to the myriad challenges of subcellular imaging using my expertise in single-molecule optical microscopy. At the same time, I propose to circumvent certain limitations (e.g., aberrations, phototoxicity, photobleaching) intrinsic to existing optical techniques by developing nanoscale magnetic imaging methods based on nitrogen-vacancy centers in diamond. My research involves significant emphases on both experimental and theoretical aspects. I am uniquely positioned for such highly interdisciplinary work, as I have trained in chemistry and physics departments and have collaborated extensively with biologists. I am seeking a tenure-track position at a Ph.D.-granting research institution and have experience teaching, tutoring, and mentoring both undergraduate and graduate students.

PHYS

Abstract Title: [*Single molecules, metamaterials, and diamond magnetometry: Novel approaches in Fourier optical microscopy*](#)

74. Kurt R. Brorsen, 405 N. Elm St., Champaign, IL 61820. kbrorsen@illinois.com, 217-300-1480; University of Oklahoma (B.S., 2008); Iowa State University (Ph.D., 2014), Prof. Mark S. Gordon, Development of electronic structure methods for large chemical systems; Postdoctoral Researcher at University of Illinois at Urbana–Champaign (2014–present), Prof. Sharon Hammes-Schiffer, Inclusion of nuclear quantum effects in quantum chemistry calculations. Department of Energy Computational Science Graduate Fellowship.

My research plan focuses on the use of computational chemistry to aid in the development of materials for the capture of gasses such as carbon dioxide and the design of electrocatalysts for renewable and sustainable energy sources. The research plan will also develop new machine-learning–based theoretical methods that are well suited to calculations on these systems. I am interested in a position at a research institution and the opportunity to mentor both graduate and undergraduate students. I would like to teach both undergraduate and graduate classes and would be excited to incorporate computational chemistry into the undergraduate curriculum in some fashion, whether directly in the classroom or in the physical chemistry lab setting.

PHYS, COMP

Abstract Title: [*Computing nuclear quantum effects with the nuclear electronic orbital approach*](#)

75. Sean C. Edington, Department of Chemistry, University of Texas at Austin, 105 E. 24th St. Stop A5300, Austin, TX 78712-1224. seanedington@gmail.com; University of Virginia (B.S., 2009); Princeton University (Ph.D., Phys Chem, 2015), Dr. Steven Bernasek and Dr. Annabella Selloni, A diode laser study of the catalytic oxidation dynamics of acetaldehyde on polycrystalline platinum; Postdoctoral Fellowship at University of Texas at Austin (2015–present), Dr. Carlos Baiz, Studying biomolecule dynamics with molecular dynamics simulations, FTIR spectroscopy, and ultrafast 2D IR spectroscopy.

www.seanedington.com

I am interested in building informative models of the chemical dynamics controlling key processes in biochemistry and catalysis. I propose to use molecular dynamics simulations in combination with a variety of vibrational spectroscopic techniques to reveal the dynamics that underpin these processes on timescales from nanoseconds to seconds. The conformational cascade that travels outward from binding sites when a protein binds its ligand(s) will be the focus of my initial research. A passionate and reflective teacher, I assisted in several physical and environmental chemistry courses, served for three years as a graduate teaching fellow, and guest lectured a large general chemistry course, among other experience. I want to inspire a profound appreciation of chemistry in undergraduates and mentor graduate students through rigorous and meaningful research projects at a research university.

PHYS, BIOL

Abstract Title: *Revealing the dynamics that control protein and biomolecule activity using FTIR and ultrafast 2DIR spectroscopy in combination with molecular dynamics simulations*

76. Brynna H. Jones, 344 Market St. E. #178, Gaithersburg, MD 20878. jone1674@umn.edu, Work: 301-975-2140, Cell: 765-729-4249; Wheaton College, Wheaton IL (B.S., Chem; B.A., Ancient Languages, 2008); University of Minnesota, Minneapolis (M.S., 2010; Ph.D., 2015), Dr. Aaron Massari, Dynamics, solvent, and reactions: Ultrafast infrared spectroscopy of Vaska's complex and its adducts; NRC Postdoctoral Associate at National Institute of Standards and Technology (2016–present), Dr. Stephan Stranick, Fluorescence imaging for materials applications. University of Minnesota Department of Chemistry Thesis Award (2016), NASA Postdoctoral Fellowship (not accepted) (2015), National Research Council Postdoctoral Research Associateship (2015), University of Minnesota Doctoral Dissertation Fellowship (2012–2013), Overend Award for Graduate Research in Physical Chemistry (University of Minnesota, 2011). <https://www.linkedin.com/in/brynna-jones-4b196212a/>

Light interacts with and influences the chemical world in a variety of ways that are both powerful in practical application and intellectually intriguing to me. I am particularly interested in using vibrational spectro-microscopy to investigate reactions at solid–liquid interfaces in environmental- and materials-relevant systems. I would like to teach and perform these investigations with undergraduates and possibly master's degree students at a four-year college or university. Having taught introductory physical science at a small university, I value excellent, research-inclusive scientific education for science and nonscience majors alike. I plan to bring chemistry, biology, geology, physics, and/or nonscience majors together into the research lab to build and design instrumentation, perform and design experiments, obtain and analyze data, and present results.

PHYS, ANYL

Abstract Title: [Wide-field super-resolution infrared microscopy for aquatic pollutant examination](#)

77. Zhou Lin, Dept. of Chemistry, Massachusetts Institute of Technology, 77 Massachusetts Ave., Bldg 6-226, Cambridge, MA 02139. zhoulin@mit.edu, 614-370-4528; University of Science and Technology of China (B.S., Chem Physics, 2009), Dr. Quanxin Li (Chem Physics), Inorganic chemistry and materials science, Sol-gel synthesis of the $12\text{CaO}-7\text{Al}_2\text{O}_3-\text{X}$ -nanoparticles and investigation of its antibacterial property; The Ohio State University (Ph.D., Chem Physics, 2015), Dr. Anne B. McCoy (Chem) and Dr. Eric Herbst (Physics and Astronomy), Theoretical and computational chemistry, Theoretical studies on the spectroscopy of astrochemically significant species and the mechanisms of relevant reactions; Postdoctoral Associate at Massachusetts Institute of Technology (2015–present), Dr. Troy A. Van Voorhis, Theoretical and computational chemistry, Construction of “black-box” theory for photochemical and photophysical processes in organic electronics using density functional theory. The Women in Chemistry Professional Development Grant, MIT Women in Chemistry, Cambridge, MA (2016); Selected Hot Topic Talk, 2015 Gordon Research Conference on Gaseous Ions: Structures, Energetics & Reactions, Galveston, TX (2015); The Presidential Fellowship, The Ohio State U (2014); The Journal of Physical Chemistry Poster Award (2013); Midwest Theoretical Chemistry Conference, Urbana–Champaign, IL (2013); Outstanding Bachelor's Thesis Award, U of Science and Technology of China (2009).

<https://www.linkedin.com/in/zhou-lin-12380517/>

<https://scholar.google.com/citations?user=FqemY3IAAAAJ&hl=en>

I am interested in understanding the electronic structures for photochemically active organic semiconductors and biological complexes, as well as their spectroscopy and dynamics, from the theoretical and computational perspective. We will construct the “black-box” tools based on *ab initio* electronic structure theory, density functional theory, and diffusion Monte Carlo, implement them to the software, and apply them to systems of interest. I hope my proposed research can attract undergraduate and graduate students in theoretical and computational chemistry. During graduate school, I have taught graduate-level quantum chemistry recitations and a series of undergraduate-level general chemistry labs. My immediate goal is to become a tenure-track faculty member in physical chemistry or chemical physics at a research-oriented university with a decent Ph.D. program.

PHYS, COMP, ENVR

Abstract Title: *Photochemical dynamics for intramolecular singlet fission in covalently-bound pentacene dimers*

78. J. Pablo Palafox-Hernandez, Chemistry Dept., The University of Kansas, 6008 Malott Hall, 1251 Wescoe Hall Dr., Lawrence, KS 66044. palafox@ku.edu, pablo.palafox49@gmail.com; The Autonomous University of Guadalajara (B.S., Chem Eng, 2001); Celaya Institute of Technology, Mexico (M.S., Chem and Petroleum Eng, 2004), Prof. Richart Vazquez, Simulation and optimization of continuous gas lift process; University of Kansas (Ph.D., Phys Chem, 2011), Prof. Brian B. Laird, Structure, thermodynamics and kinetics of chemically heterogeneous interfaces; Postdoctoral Researcher at Duke University (2011–2012), Patrick Charbonneau, Effect of the wall structure in the interfacial free energy for hard-sphere fluids; Institute for Frontier Materials (2012–2015), Tiffany Walsh, Bio-nanocombinatorics to achieve precisely-assembled multicomponent, functional hybrid nanomaterials; Postdoctoral Researcher at Center for Environmentally Beneficial Catalysis CEBC, The University of Kansas (2015–present), Brian B. Laird, Sustainable chemical innovations by an integrated design approach. Best Oral Presentation Award, Symposium A: Modeling and Theory-Driven Design 2013 of Soft Materials, MRS Boston MA; The Paul and Helen Gilles Award in Physical Chemistry (Superior academic performance and research accomplishments by an advanced doctoral student), KU Lawrence, KS (2009); CONACYT Fellowship (Mexican equivalent to NSF) ITC Celaya, Gto. México (2002–2004); Graduated with honors and Best GPA in Chemistry Department UAG, Guadalajara, Jal. México (2001).

https://www.researchgate.net/profile/Pablo_Palafox2

<https://cpe.ku.edu/pablo-palafox>

My career goal is to use my experience and passion for science in the training of future scientists and well-informed citizens. Following a nonlinear path, I gained an interdisciplinary background, with a Ph.D. in Computational Physical Chemistry (emphasis in material science), and M.S. and B.S. degrees in Chemical Engineering. Throughout my formation, I have had to tackle a highly diverse array of educational and research problems. I can count considerable international experiences; I have performed teaching and research in Mexico, the United States, and Australia, producing meaningful and influential results—several of my mentored students have won recognition at regional, national, and international meetings. I greatly enjoy teaching and collaborating closely with the students to help them to achieve their full potential.

PHYS, COMP, MAT SCIENCE

Abstract Title: *Crystal orientation dependence of heterogeneous nucleation at the Cu-Pb solid-liquid interface*

79. Samuel C. Perry, Dept. of Chemistry, McGill University, 801 Rue Sherbrooke O, Montreal, QC, H3A 0B8. samuel.perry@mcgill.ca; University of Southampton (MChem, 2012; Ph.D., 2016), Dr. Guy Denuault, Transient studies at microelectrodes; Postdoctoral Research Fellow at McGill University (2016–present), Dr. Janine Mauzeroll, Electrochemistry, including corrosion, ECL, and biosensors. Registration Bursary from the ISE (£200); Travel Grant from the RSC (£400); Faraday Division Conference Fund (£700); IOP Research Student Conference Fund (£300); Scholarship grant, sp3 scholarship for achieving one of the ten highest average exam scores of the year. (£3,000).

<http://bioelectrochemistry.mcgill.ca/>

My primary area of interest centers on the use of microelectrodes as a tool for chemical analysis. I have a great deal of experience in this area, both in terms of bulk electroanalytical methods and high-precision scanning probe techniques, such as scanning electrochemical microscopy (SECM). I am currently working as a Postdoctoral Researcher at McGill University, where I am involved in a number of projects, including finite element simulation of corroding metals, ECL, and the fabrication of novel enzymatic biosensors. I already have experience with teaching and supervision, having taught a number of classes in chemistry modules to undergraduate and graduate students over the course of my Ph.D. and postdoctoral work. I am looking forward to the opportunity to teach a complete electrochemical module at a university to undergraduate or graduate students.

ANYL, PHYS

Abstract Title: [*Localized detection of D-serine by using an enzymatic amperometric biosensor and scanning electrochemical microscopy*](#)

80. Christopher C. Rich, Dept. of Chemistry, Colorado State University, 200 West Lake St., Fort Collins, CO, 80523. richcc@colostate.edu; Stonehill College (B.S., ACS Certified, 2008); Washington State University (Ph.D., 2013), Dr. Jeanne L. McHale, Using Raman spectroscopy to probe the internal structure and excitonic properties of light harvesting aggregates of tetra(sulfonatophenyl)porphyrin; Postdoctoral Researcher (2013–2016) and Research Scientist (2016–present) at Colorado State University, Dr. Amber T. Krummel, Measurement of absolute molecular orientation of dyes at solar energy interfaces and in molecular aggregates using heterodyne-detected vibrational sum frequency generation spectroscopy.

I am a physical chemist interested in uncovering the underlying excitonic and vibrational photophysics associated with light-harvesting molecular aggregates using a combination of linear and nonlinear spectroscopy and microscopy techniques. In my current work, I have designed and implemented a heterodyne-detected vibrational sum frequency generation spectrometer to determine the absolute orientation of molecules in various noncentrosymmetric media. I hope to build off skills I have gained to take part in designing new spectroscopy and microscopy techniques, which may interrogate the relationship among molecular organization, exciton delocalization, and exciton transport. My ambition is join the faculty at a research-intensive university where I may develop a robust and collaborative research program while mentoring and teaching graduate and undergraduate students and postdocs.

PHYS, COLL

Abstract Title: [*Revealing the excitonic and structural properties of light-harvesting molecular assemblies through electronic-vibrational spectroscopy*](#)

81. Ryan M. Richard, Ames National Laboratory. ryanmrichard1@gmail.com; Cleveland State University (B.S., 2008); The Ohio State University (Ph.D., 2013), Dr. John M. Herbert, The many-body expansion; Postdoctoral Researcher at the Georgia Institute of Technology (2013–2017), Dr. C. David Sherrill, Parallelizing computational chemistry packages; Postdoctoral Researcher at Ames National Laboratory (2017–present), Dr. Theresa Windus, Parallelizing computational chemistry packages. Finalist for the Emerging Technology in Computational Chemistry Symposium at the 252nd America Chemical Society National Meeting and Exposition (2016); The Ohio State University Graduate School Fellowship (2008); Best Undergraduate Presentation, Cleveland Section of the American Chemical Society Meeting in Minature (2007); Cleveland State University Honors Program Scholarship (2004).

Ryan aims to find a professorship at a graduate degree–granting institution. He is particularly interested in the opportunity to teach physical, quantum, or computational chemistry, or all three, as well as electronic structure theory. His planned research will use quantum chemistry to help design and increase our understanding of molecular magnets. Integral to this research will be his code, Pulsar. It is Ryan’s belief that, similar to other emerging quantum chemistry software, Pulsar offers unique opportunities for teaching, owing to its accessibility from high-level languages. In particular, with little formal coding skill, students can write their own implementations of most quantum chemistry theories. Such exercises bridge the gap between the abstract theories of quantum mechanics and the more concrete results of chemistry.

PHYS, COMP

Abstract Title: [*Leveraging a computational chemistry app-store for both teaching and researching chemistry*](#)

82. Handan Acar, 5020 S. Lake Shore Dr., N3302, Chicago, IL 60615. hacar@uchicago.edu, 617-416-7504; Gazi University, Turkey (B.S., 2006); Ankara University, Turkey (M.S., 2008); Bilkent University, Turkey (Ph.D., Mat. Sci. Nano., 2013), Dr. M. O. Guler, Template directed synthesis of one-dimensional inorganic nanostructures and applications; Postdoctoral Researcher at University of Chicago (present) (IME), Dr. Matthew Tirrell, Peptide amphiphiles for cancer treatment.

My research is on chemical methodologies to tune the supramolecular interactions of self-assembling molecules to surmount the key challenges for peptide-based therapeutics, diagnostics, and delivery platforms. I have developed a self-assembled nanoparticle platform for cancer treatment. I taught Fundamentals of Thermodynamics of Mechanical Engineering in Spring 2014. I want to establish a lab at a prestigious research university, working on designing materials from a molecular perspective for translational clinical technologies. A specific emphasis will be placed on using an interdisciplinary approach from physical and synthetic chemistry for therapeutic and diagnostic applications. I also want to teach at the undergraduate and graduate levels.

PMSE, MEDI, BIOT

Abstract Title: *Engineering the molecular interactions for biomedical applications*

83. Pengfei Cao, Chemical Sciences Division, Oak Ridge National Laboratory. caop@ornl.gov, 330-322-9619; Tianjin University, Tianjin, China, (B.E., Appl Chem, 2008; M.S., Polymer Chem and Physics, 2010), Yu Chen; Case Western Reserve University, Cleveland (Ph.D., Macromolecular Sci and Eng, 2015), Rigoberto Advincula; Postdoctoral Research Associate at Chemical Sciences Division, Oak Ridge National Laboratory (present). Publications include: *Angew. Chem. Inter. Ed.*, *Macromolecules*, *ACS Nano*, *Chem. Commun.*, *Nanoscale* and *ACS Macro Letters*; 20 journal papers (12 as 1st author), 2 book chapters (1 as 1st author); refereed several journals, including *Advanced Functional Materials*, *Small*, *Reactive and Functional Polymer*, *Advanced Material Interfaces*, and *Polymer Chemistry*.

<https://www.ornl.gov/staff-profile/pengfei-cao>

<https://scholar.google.com/citations?user=nIbBMUQAAAAJ&hl=en>

I focus on synthesizing and characterizing polymers with unconventional architectures, including a single Li-ion conducting polymer electrolytes and comb-like polymer binder for Li-ion battery applications and a synthetic self-healing polymer membrane for CO₂ separation. I've a strong publication record and significant classroom and lab teaching experience with both undergrad and grad students. I mentor several highly productive M.S. students. I seek a tenure-track position in a Ph.D. program in chem, polymer sci and eng, chem eng and mat sci and eng. I'd like to expand research on polymer synthesis for fundamental study and applications in energy storage, nanomedicine, and gas separation and offer courses such as polymer chem, orgn chem, polymer physics, polymer for oil–gas industry, and polymer for energy storage, at both grad and undergrad levels, plus support the existing curriculum.

PMSE, POLY

Abstract Title: *Synthetic polymers with unconventional architectures for energy storage*

84. Melanie Ecker, Dept. of Materials Science and Engineering, University of Texas at Dallas, 800 W. Campbell Rd., Richardson, TX 75080. melanie.ecker@utdallas.edu; Freie Universität Berlin, Germany (Intermediate Diploma in Chem equivalent to B.S., 2006; Diploma in Chem equivalent to M.S., 2010), Dr. Laura Hartmann, Sequence-defined insertion of anionic groups into linear and monodisperse poly(amidomines); Freie Universität Berlin, Germany, (Ph.D., 2015), Dr. Thorsten Pretsch, Development, characterization and durability of switchable information carriers based on shape memory polymers; Postdoctoral Studies at University of Texas at Dallas (2015–present), Dr. Walter Voit, Shape memory polymers as substrate for bioelectronic devices.

<https://www.linkedin.com/in/melanie-ecker-54948196/>

I have a strong background and expertise in polymer chemistry and the structure–property relationship of polymeric materials, including shape memory polymers. Postdoctoral research included developing and characterizing self-softening shape memory polymers as substrates for flexible bioelectronics. Long-term career objectives: become an independent researcher investigating polymeric materials as substrates for biomedical devices, especially for peripheral neural interfaces. Understanding the enteric nervous system particularly interests me. I've worked with researchers from multidisciplinary backgrounds, produced peer-reviewed publications, and presented my results at numerous national and international conferences. I completed a course for supervisors and managers and am currently enrolled in a teaching certificate program. I am also mentoring a group of undergrad and graduate students.

POLY, PMSE

Abstract Title: [*Self-softening shape memory polymers as a substrate for bioelectronic devices*](#)

85. Michael G. Mazzotta, Dept. of Chemistry, Purdue University, 560 Oval Dr., West Lafayette, IN 47905. mmazzott@purdue.edu; Eastern Kentucky University (B.S., magna cum laude, 2012); Purdue University, (Ph.D., anticipated 2017), Prof. Jonathan J. Wilker, Synthesis, characterization and catalysis of dioxorhenium pincer complexes; Toughening biomimetic adhesives through H-bonding interactions. Charles Cameron Professional Development Award; Emerson Kampen Fellowship; Ian P. Rothwell Distinguished Inorganic Seminar Award; Frederick N. Andrews Fellowship; Phi Kappa Phi Graduate Fellowship.

www.linkedin.com/in/mikemazzotta

Having had the privilege of performing research in both catalysis and biomaterials, I have realized that enzymes are a marriage of these two fields. Enzymes are biopolymers of profound structural complexity, housing active sites that are often at the peak of catalytic efficiency and selectivity. I am currently seeking a postdoctoral position in biocatalysis, where I would like to learn more about how the subtleties in protein structure affect reactivity, and how alternative catalytic functions can be coaxed out of an enzyme. Mentoring students has been a particularly enjoyable and rewarding component of research; thus, I'm aspiring to teach and lead a research group at an R-1 institution. Being able to journey through the intricacies of life's molecular machinery with a team of motivated undergraduate, graduate, and postdoctoral researchers is my dream job.

PMSE, POLY, INOR

Abstract Title: *Balancing strength and ductility in biomimetic adhesives through breakable bonds*

86. Davoud Mozhdehi, Dept. of Biomedical Engineering, Duke University, 101 Science Dr., Durham, NC 27708. davoud.mozhdehi@duke.edu; Sharif University of Technology (B.S., Pure Chem, 2008); University of California, Irvine (Ph.D., 2015), Dr. Zhibin Guan, Transient supramolecular interactions for templating peptide folding and designing new self-healing polymers; Postdoctoral Associate at Research Triangle Materials Research Science and Engineering Center, Dept. of Biomedical Engineering at Duke University (2015–present), Dr. Ashutosh Chilkoti, Synthesis of smart biohybrid materials through post-translational modification of biopolymers. Teaching Excellence & Service to Academic Community (2014); UCI Pedagogical Fellowship (2013); UCI Department of Chemistry Teaching Award (2012).
<https://scholar.google.com/citations?user=Dg-e23QAAAAJ&hl=en>
<https://www.linkedin.com/in/dmozhdeh/>

My research interests are at the interface of chemistry, biology, and materials science. My laboratory will use an interdisciplinary approach to create novel, smart materials to address challenging questions in those fields. In particular, we will leverage advances in synthetic chemistry and chemical biology to create novel, hybrid biomaterials to manipulate biological systems. Inspired by adaptive biological materials, we will also focus on creating smart, high-performance materials for engineering applications. Teaching and mentoring the next generation of scientists and engineers will be important components of my academic endeavors. Motivated by my training as a UC Irvine pedagogical fellow, I will curate an inclusive, active learning environment to ensure the success of students with different learning styles in my classes.

POLY, PMSE, BIOL, ORGN

Abstract Title: *Harnessing the power of post-translational modifications for materials science and engineering*

87. Cornelia Rosu. cornelia.rosu@mse.gatech.edu; Al. I. Cuza University of Iasi, Romania (B.S., 1996); Louisiana State University (M.S., 2010), Paul Russo, William Daly, and Ioan I. Negulescu (HUEC), Recent advances in glylons science; Louisiana State University, (Ph.D., 2013), Paul Russo, Silica polypeptide-based colloids: Physical properties and novel materials; Research Associate at Louisiana State University (2013–2014), Dr. Paul Russo, Polypeptide liquid crystals; Postdoctoral Fellow at Georgia Institute of Technology (2014–2016), Dr. Elsa Reichmanis (ChBE), Protein-assisted organization of conjugated polymers into crystalline structures; Postdoctoral Fellow at Georgia Institute of Technology (2016–present), Dr. Dennis Hess and Dr. Victor Breedveld, Polymeric surface modification to manage moisture and heat transport. Chemistry and Physics teacher, Romania (1996–2007). The Excellence in Polymer Research Award (ACS POLY Division, 2013); Dow Chemical Excellence Award (Department of Chemistry, LSU, 2011).

Cornelia Rosu, a postdoc in chem and biomolecular engineering at Georgia Institute of Technology (GIT), held previous positions at GIT School of Materials Science and Engineering and the Chemistry Dept. at LSU. After earning her B.S. degree, she taught chemistry and physics in Romania for a few years, then earned her M.S. and Ph.D. in chemistry from LSU. She received the ACS Excellence in Polymer Research Award and Dow Chemical Excellence Award. Research interests encompass polymers and complex fluids, with a focus on designing soft materials with tunable properties, as well as engineering bioderived electroactive materials for use in bioelectronics, implantable and wearable devices, or sensors for detecting the quality of packaged foods. A member of ACS and the American Polypeptide Society, she wants to teach undergrad and grad-level classes in chemistry, colloids, and polymer science.

PMSE, COLL, POLY, PHYS

Abstract Title: [Engineering hierarchical and functional structures with an elegant tool: Polypeptides](#)

88. Monirosadat (Sanaz) Sadati, 5640 S. Ellis Ave., ERC 251, Chicago, IL 60637.
msadati@uchicago.edu, 857-756 0747; Amirkabir University of Technology, Tehran, Iran (B.S., Polymer Eng, 2000), Prof. Naser Mohammadi, Prediction of scratch resistance of acrylic-melamine clear coats on the basis of fracture energy; Amirkabir University of Technology, (M.S., Polymer Eng, 2003), Prof. Naser Mohammadi, Gel spinning of starch; ETH Zürich, Switzerland (Ph.D. in Mat Sci, 2012), Prof. Hans Christian Öttinger, Complex flow of linear and branched polyethylene melts in a cross-slot flow channel: Birefringence, particle tracking, data analysis, and rheological modeling; Graduate Researcher at ETH Zürich, Polymer Physics Institute (2007–2012). Prof. Hans Christian Öttinger, (i) Modified the lubricated optical rheometer to improve flow stability for the study of two-dimensional complex flows of polyethylene melts (ii) Verified the two dimensionality of the flow using particle image velocimetry (iii) Performed point-wise and field-wise flow-induced birefringence and particle tracking techniques, respectively to collect stress and velocity fields and analyzed the data (iv) Established a regularization technique based on high order finite element approximation to reconstruct accurate full field kinematics from noisy experimental data (v) Examined the performance of eXtended Pom-Pom model for LDPE and HDPE using numerical simulations and implementing the regularized experimental flow kinematics in two-dimensional complex flows; Postdoctoral Researcher at Harvard University (2012–2014), Prof. Jeffrey Fredberg, (i) Developed an assay to study physical forces and rheology of cellular collective in contraction channels (ii) Designed and built a device to apply intercellular shear deformation on cellular collective and evaluated the response of the living cell; Postdoctoral Researcher at The University of Chicago and Argonne National Laboratory (2014–present), Prof. Juan J. de Pablo, (i) Studied dynamics of linear and branched DNA molecules in microfluidic channels (ii) Explored the molecular organization of LCs at LC-air interface and under the influence of ions at LC-water interfaces using synchrotron X-ray reflectivity. (iii) Developed a LC based sensor to detect early-stage aggregation of polypeptides involved in neurodegenerative diseases such as Alzheimer (Published in *Advanced Functional Materials* (2015) and featured on the Journal's cover) (iv) Stabilized blue phase liquid crystals using polymers at room temperature. Swiss National Science Foundation Prospective Researchers Award (\$57,200; 2012); Swiss National Science Foundation Advanced Postdoc. Mobility Award (\$64k; 2013).

I am interested in exploring structure–rheology–property relationships of polymeric materials and lyotropic and biological *liquid* crystalline mesophases to find new routes for engineering new functional soft materials with tunable properties for biomedical, drug delivery, photonics, and water desalination applications. Moreover, building on my previous work and background, I am particularly interested in the rheological and processing aspects of additive manufacturing to develop strategies for materials optimization. With the background in polymer engineering and physics, I have a strong foundation on materials science, in particular polymer science–related courses including polymer physics, polymer chemistry, rheology, and characterization.

PMSE, COLL

Abstract Title: [Complex fluids and anisotropic liquids for intelligent molecular engineering and material design: Structure-rheology-property relationships](#)

89. Andres Mauricio Tibabuzo Perdomo,

Purdue University, Dept. of Chemistry, 560 Oval Dr., West Lafayette, IN 47907.

atibabuz@purdue.edu, 765-479-5803; Universidad de los Andes (B.S., Bio, 2013); Purdue University (Ph.D., 2019), Dr. Jonathan J. Wilker, Understanding the origins of bioadhesion in marine organisms. Applied Management Principles mini-MBA Award (2017); Charles Cameron Professional Development Award, Purdue University (2016); Frederick N. Andrews Fellowship, Purdue University, (2014–2016); National Contest Otto de Greiff, Best undergraduate thesis (2013).

I'm a biologist currently working toward a Ph.D. in Chemistry at Purdue. I'm interested in natural compounds, bioprospection, and biomimetics, with a special interest in venomous animals. Back in my home country, Colombia, I worked on a project characterizing how the physicochemical properties of membranes affect the enzymatic activity of venom phospholipases from the snakes *Bothrops asper* and *Crotalus durissus cumanensis*. Currently at Purdue, I work in the Wilker lab characterizing the cement that oysters produce. This cement is an inorganic–organic composite material that is able to hold together oyster reefs in extreme conditions, such as cycling through dry and wet environments—something that we still cannot achieve with man-made materials. I am very interested in discovering and applying the vast array of compounds that nature produces, turning them into tangible tools.

BIOT

Abstract Title: [*Understanding marine bio-adhesion: Characterization of the eastern oyster cement*](#)

90. Jeffrey R. Vieregg, Institute for Molecular Engineering, University of Chicago, ERC 108, 5640 S. Ellis Ave., Chicago, IL 60637. jvieregg@uchicago.edu; Massachusetts Institute of Technology (S.B., Physics, 2001); University of California, Berkeley (M.A., 2004; Ph.D., 2007), Dr. Ignacio Tinoco and Dr. Carlos Bustamante (Physics), Single molecule RNA folding studied with optical trapping; Postdoctoral Researcher at Department of Bioengineering, California Institute of Technology (2008–2013), Dr. Niles Pierce, Engineering conformation-switching nucleic acid nanodevices for imaging and control of gene expression; Senior Research Scientist at Institute for Molecular Engineering, University of Chicago (2013–present), Prof. Matthew Tirrell, Self-assembly of nucleic acids by polyelectrolyte complexation, nucleic acid templated catalysis, and protein assembly. NSF Graduate Research Fellowship; UCBREP Graduate Research and Education in Adaptive Biotechnology Training Grant.

<http://home.uchicago.edu/~jvieregg/>

Nucleic acid hybridization is a molecular recognition code that has been optimized by millions of years of evolution. After decades of study, we have reached the point where we can predict the thermodynamics and kinetics of nucleic acid folding with reasonable accuracy, as evidenced by the complex constructions of structural DNA nanotechnology. I want to use this powerful toolbox to create functional nucleic acid nanodevices that perform chemical transformations and assemble other biomolecules with nanometer spatial resolution inside living cells and organisms. By constructing conformation-switching structures, we can couple chemical responses to genetic and environmental changes, enabling a powerful new generation of sensors and therapeutic interventions. I hope to teach and mentor undergraduate and graduate students at a research-focused university.

BIOL, PMSE, BIOT

Abstract Title: *Programming self-assembly and function at multiple scales with nucleic acids*

91. Weinan Xu, Johns Hopkins University. weinanxu@gmail.com; Donghua University, China (B.S., Polymer Sci and Eng, 2011); Georgia Institute of Technology (Ph.D., Mat Sci and Eng, 2015), Vladimir. V. Tsukruk, Responsive micro- and nano-structures through interfacial assembly of star polymers; Postdoctoral Fellow at Johns Hopkins University, Dept. Chem & Biomolecular Eng (2016–present), David H. Gracias, Fabrication of 3-D micro- and nano-structures from 2-D materials, including graphene and transition metal dichalcogenides.

My research interests focus on responsive soft 3-D micro/nanostructures with the abilities to adapt and respond to external stimuli and their applications in biosensing, drug delivery, and flexible electronics. The building blocks for the 3-D structures include, but are not limited to, responsive polymers, nanoparticles, and 2-D nanomaterials. Fabrication of the 3-D structures relies on the combination of bottom-up synthesis and top-down fabrication techniques; moreover, self-assembly, self-folding, and 3-D printing are also used to achieve highly ordered 3-D structures.

PMSE, POLY, COLL

Abstract Title: *Three-dimensional responsive soft micro/nano-structures for biomedical and electronic applications*

Technical Abstracts AEI 2017

AEI 1

Identification of antimicrobial peptide from soy protein

Ning Xiang¹, xiangn@purdue.edu, Yuan Lyu¹, Xiao Zhu³, Arun Bhunia⁴, Ganesan Narsimhan².

(1) Agricultural and Biological Engineering, Purdue University, West Lafayette, Indiana, United States (2) Dept of Agric Biological Eng, Purdue University, West Lafayette, Indiana, United States (3) Rosen Center for Advanced Computing, Purdue University, West Lafayette, Indiana, United States (4) Food Science, Purdue University, West Lafayette, Indiana, United States

Antimicrobial peptides (AMPs) inactivate microbial cells through pore formation in cell membrane. Because of their different mode of action compared to antibiotics, AMPs can be effectively used to combat drug resistant bacteria in human health. In this research, we developed a methodology based on mechanistic evaluation of peptide-lipid bilayer interaction to identify AMPs from soy protein. Initial screening of peptide segments from soy glycinin (11S) and soy β -conglycinin (7S) subunits was based on their hydrophobicity, hydrophobic moment and net charge. Out of several candidates chosen from the initial screening, two peptides satisfied the criteria for antimicrobial activity, viz. (i) lipid-peptide binding in surface state and (ii) pore formation in transmembrane state of the aggregate, as evaluated by all-atom molecular dynamic (MD) simulation. Their antimicrobial activities against *Listeria monocytogenes* and *E.coli* were further confirmed by spot-on-lawn test. This methodology is also applicable for identification of AMPs from any protein.

AEI 2

Fluorescamine-based screening of protein-protein interfaces

Jonathan Ashby, jashby@mtholyoke.edu. Mount Holyoke College, South Hadley, Massachusetts, United States

Interactions between proteins and other biological macromolecules in the body are responsible for a variety of cellular functions. In cancer and other diseases, some protein-protein interactions have been tied to tumorigenesis, metathesis, and other adverse processes. Understanding both the identity and the nature of these interactions is key to being able to more accurately predict future interactions as well as develop potential treatments to either interfere or simulate these interactions, depending on the desired outcome of the treatment.

Although the identities of many of these interactions are known, the interface in which the interactions occur has been harder to determine and predict. Many commonly used experiments for determining protein structure, such as x-ray crystallography, are often highly-time consuming, require large amounts of analyte, and may not properly emulate physiological conditions. Instead, usage of amino acid-specific tags followed by mass spectrometric analysis can be used for determination of protein tertiary structure, as well as protein-protein interactions. Fluorescamine is a lysine and arginine specific tag that has the benefits of being rapid-reacting and capable of functioning under physiological conditions. As a result, it can be used for both analysis of stable, rigid-body protein-protein interactions, as well as more transient interactions. Single proteins as well as known protein-protein pairs were incubated with fluorescamine, and digested with chymotrypsin. The resulting peptide digests were analyzed via mass spectrometry in order to identify the location of fluorescamine tags. By identifying the identity of particular amino acids as solvent accessible or buried (either within the protein structure or within the protein-protein interface) and comparing these findings to that of well-characterized pairs, the effectiveness of using this method for determining the protein-protein interface can be assessed.

AEI 3

Label-free optical biomolecular sensing using single wall carbon nanotubes

Juyao Dong, juyao@mit.edu. Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States

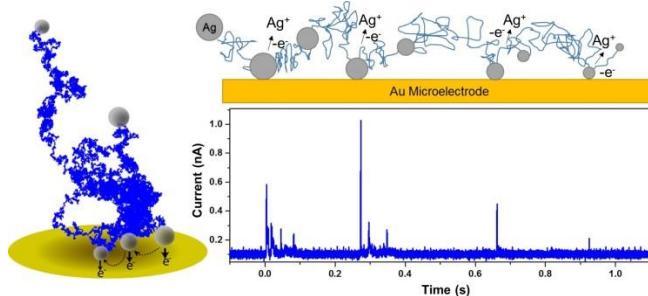
In this presentation, a multiplexed molecular detection platform based on the fluorescent emissions of single wall carbon nanotubes will be presented. The carbon nanotubes are non-covalently modified with chelating group nitrilotriacetic acid and Cu 2+ ions. By conjugating a recognition moiety with the Cu2+ ion, the carbon nanotubes are capable of specifically recognize the target analyte transduced by their changed fluorescence emission properties. Moreover, we have developed a miniature mircorarray system to integrate multiple recognition sites onto a small area of glassslide. Using only a few microliter of the sample, we are able to quickly detect multiple analytes using our nanosensor platform. The label-free system will be of great potential for product quality control and clinical diagnosing applications in the future.

Effect of solution viscosity on multi-electron transfer from repeated collisions of a single Ag nanoparticle on an Au electrode

Donald A. Robinson, donny.robinson@utah.edu, **Yuwen Liu**, **Martin A. Edwards**, **Henry S. White**. Chemistry, University of Utah, Salt Lake City, Utah, United States

Electrochemical dissolution of a 70 nm radius citrate-stabilized Ag nanoparticle on an Au microelectrode has been observed to produce multiple sharp peaks in the resulting oxidation current monitored over time, with roughly 1-100 ms durations in between each peak. The multiplicity of the peak behavior was previously interpreted to arise from multiple collisions of the same Ag nanoparticle on the electrode surface while simultaneously undergoing a partial oxidation/dissolution event upon each collision.

Here, the role of Brownian motion on nanoparticle collision frequency is investigated by performing single nanoparticle collision experiments in 3 different glycerol/water mixtures with viscosities of 0.96, 1.9, and 4.5 cP. The motion-dependent features of the single-nanoparticle oxidation signal, such as peak currents and peak frequencies, were averaged together from 160 particle tracks per solution viscosity studied. The average motion-dependent parameters follow distinct trends as a function of the solution viscosity. Similar trends are observed from simulated current vs time traces that were generated for single Ag nanoparticles following a 3D random-walk model based on the theory of Brownian motion while simultaneously accounting for the collision-dependent current resulting from electrochemical Ag dissolution. These trends are explained based on nanoparticle/electrode collision frequencies obtained in random-walk simulations and analytical solutions derived from the basic theory of random walk. The findings support a microscopic model of electrochemical kinetics that unites Einstein's theory of Brownian motion with the collisional dependence of reactions involving multi-electron transfer.



AEI 5

Designing food analysis experiments for the promotion of critical thinking in the instrumental analysis laboratory

Ornella Sathoud², osathoud@udel.edu, Karl S. Booksh¹, Jacqueline L. Hilsenbeck-Fajardo¹, Daniel Kraiter¹, Collin Maunz¹. (1) University of Delaware, Newark, Delaware, United States
(2) Chemistry and Biochemistry, University of Delaware, Newark, Delaware, United States

Critical thinking is defined as: the objective analysis and evaluation of an issue in order to form a judgment. Critical thinking has been categorized as one of the skills to have in order to be successful academically and professionally. Throughout their academic career, some students will compartmentalize the knowledge and/or skills acquired, which could prevent them from using that knowledge when needed in a setting different from the one they acquired it or could fail to recognize that they have already acquired the knowledge and/or skills needed to solve the task at hand. In this report we are addressing the difficulties students display to translate theory to practice, which could be explained by a lack of activities targeting the enhancement of critical thinking. This phenomenon is well observed among STEM student and in this presentation we focused on Junior and Senior chemistry students taking instrumental analysis laboratory. To address the issue of critical thinking and knowledge compartmentalization, we designed a series of laboratory projects based on problem based learning to help promote students critical thinking in order to decompartmentalize knowledge and a rubric used to assess the students growth.

AEI 6

Novel characterization of block copolymer and biopolymer matrices using fluorescence microscopy methods

Khanh Hoa Tran Ba, khtranba@gmail.com. Chemistry, Columbia University, New York, New York, United States

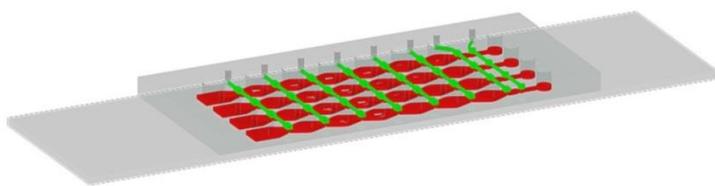
In recent years, phase-separated block copolymer films and microporous biopolymer hydrogels have attracted considerable attention as novel materials for a variety of applications. The interests primarily stem from their unique material properties such as their uniform shapes of tunable diameters, well-controlled stiffness and porosity, and biocompatibility. Applications of block copolymers matrices include masks for photolithography, membranes for separation and sensing, substrates for catalysis, and materials for energy conversion and storage. On the other hand, biopolymer hydrogels have been primarily applied in tissue engineering, biotechnology and fundamental biophysical studies. Unfortunately, sub-optimum performance characteristics in these applications are currently observed which are likely causes by our still limited understanding of the material properties. Thus, my research is devoted to overcome these limitations by fully characterize these polymer matrices using novel fluorescence microscopy methods. First, single-molecule tracking studies of a typical cylinder-forming block copolymer, polystyrene-*block*-poly(ethylene oxide), is described. Single-molecule tracking allows the measurement of the solvent-swollen microdomain orientation, order and diameter by following the diffusive motion of individual fluorescent probe molecules dominantly partitioned into the poly(ethylene oxide) microdomains. The long-range microdomain connectivity could be also assessed by probing the recovery of the fluorescent intensity in the fluorescence-recovery-after-photobleaching measurements. Second, simultaneous confocal microscopy and rheology methods were employed to probe the fibrillogenesis of type I collagen hydrogels through the sol-gel transition and to investigate their shear deformation dynamics. The multi-modal approach allows the evolving microstructure with the evolving viscoelastic properties on the fibril and network length scales to be directly correlated, the rheological gel-point and fiber diameters to be determined, and non-affine network deformations prior to fiber breaking upon application of shear stress to be observed. The results of my research reveals important novel material properties of block copolymers and biopolymer matrices and thus will provide guidance to synthesize and optimize these polymers for their intended applications.

Microfluidic magnetic bead ELISA streamlined with pneumatic valves

Yang Yang¹, yangy@ku.edu, **Yong Zeng**^{1,2}. (1) Department of Chemistry, University of Kansas, Lawrence, Kansas, United States (2) University of Kansas Cancer Center, Kansas City, Kansas, United States

Enzyme-linked immunosorbent assay (ELISA) is a gold standard for quantitative detection of protein biomarkers. Conventional ELISA is based on single solid surface (e.g. a well-plate) that requires multiple times washing and pipetting to remove residual reagents and costly instrumentation (e.g. plate reader).

By employing the microfluidic technique, we have developed a magnetic bead and on-chip valve based ELISA to achieve expedient, low-cost, sensitive and pipette-free washing protein detection. The microfluidic chip consists of a pneumatic layer and a flow layer. The pneumatic layer is used to control on-chip valves. After the incubation of beads and sample, washing buffer is added into the following chamber with higher liquid surface level. When the valve is open, the washing buffer will rush into the remainder, while the beads will be pulled into the next chamber by a magnet. The appliance of communicating vessel principle enables the chip to rapidly isolate magnetic beads from the remainder by hydrodynamic flow without pipetting or any immiscible barrier. Moreover, the fluorescence signals are generated in a relatively small incubation chamber on the chip to increase sensitivity. Our method can detect sub-nanograms per milliliter of carcinoembryonic antigen (CEA). Compared to standard ELISA, our method needs less washing and sample volume. Furthermore, this microfluidic chip holds the potential to isolate other biomolecules including exosomes for cancer diagnosis. In a nutshell, this expedient, low-cost, sensitive and pipette-free washing method holds promising potential for point-of-care tests of cancer.



The bi-layer microfluidic chip. Green: pneumatic layer for controlling on-chip valves. Red: flow layer for incubation and washing.

AEI 8

Developing new tools for the study of *O*-GlcNAc transferase in disease

*Sara E. Martin*¹, *sara_martin2@hms.harvard.edu*, *Damien Y. Duveau*², *John Janetzko*¹, *Zhi W. Tan*¹, *Frederick A. Moss*¹, *Harri Itkonen*¹, *Piotrek Sliz*³, *Michael B. Lazarus*⁴, *Craig J. Thomas*², *Suzanne Walker*¹. (1) Harvard Institutes of Medicine, Room 1013, Harvard Medical School, Boston, Massachusetts, United States (2) NIH Chemical Genomics Center, Rockville, Maryland, United States (3) Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, Massachusetts, United States (4) Pharmacological Sciences, Mount Sinai School of Medicine, New York, New York, United States

O-Linked *N*-acetylglucosamine transferase (OGT) is responsible for the addition of β -*N*-acetylglucosamine (GlcNAc) to over 1,000 proteins in mammalian cells, and the addition of these *O*-GlcNAc groups to target proteins has been shown to affect localization, stability, enzymatic activity, and interactions with other biomolecules. Misregulation of OGT has been linked to cancer, diabetes, heart disease, and Alzheimer's disease. However, studies of how OGT misregulation contributes to disease have been limited, in part because fast-acting chemical tools to manipulate OGT activity in cells have remained elusive. SAR efforts have led to a series of probe compounds, some of which exhibit nanomolar Kds, are cell permeable, and exhibit no notable toxicity. Crystal structures of several cocomplexes reveal that the quinolinone-6-sulfonamide portion of the molecules serves as a uridine mimic. These inhibitors make possible future studies to elucidate the role of OGT in disease pathology and to test whether OGT inhibition may offer a therapeutic benefit. In my independent career, I hope to study the chemical biology of glycosyltransferases involved in bacterial cell wall biosynthesis and to teach classes at the interface of chemistry and biology.

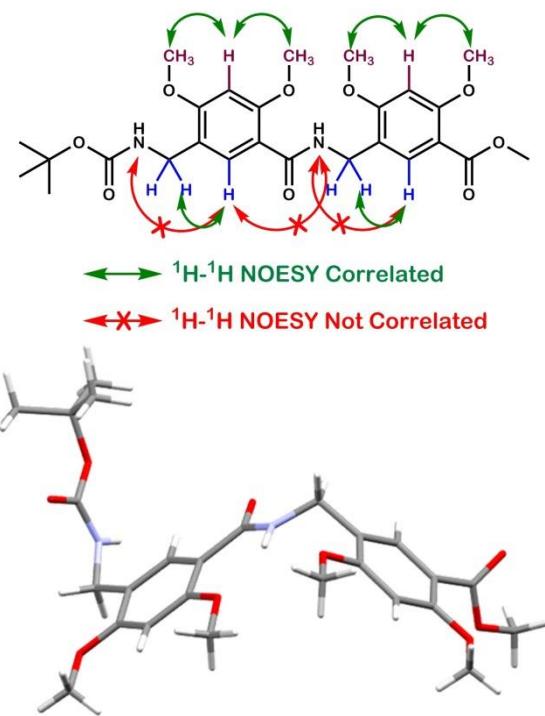
MAMBA: Hydrogen bond organized beta-strand peptidomimetics

Joseph W. Meisel, *jwm5hd@umsl.edu*, **Andrew Hamilton**. Department of Chemistry, New York University, New York, New York, United States

Novel synthetic agents designed to target protein-protein interactions (PPIs) and protein-membrane interactions (PMIs) provide an alternative therapeutic approach where traditional drug discovery methods have been unsuccessful. Small-molecule organic compounds that recapitulate the features of short peptides (peptidomimetics) and larger protein surfaces (proteomimetics) may be used as tools to guide drug discovery or as drug candidates themselves.

The research presented here involves the design, synthesis, and characterization of peptidomimetic and proteomimetic compounds that target PPIs and PMIs by folding into predicted structures and displaying functional groups with a chemical density and diversity that rivals their biological counterparts. Hydrogen bond organized derivatives of the dipeptide mimetic *meta*-aminomethylbenzoic acid (MAMBA) were synthesized in multi-gram quantities with facile purification techniques and good yield from the commodity chemical beta-resorcylic acid. The MAMBA monomers were amenable to solution and solid phase coupling methodologies.

MAMBA oligomers were characterized by NMR spectroscopy, mass spectrometry, and X-ray diffraction techniques. The MAMBA scaffold was shown to have the predicted hydrogen bonding pattern in solution and solid phases and was shown to template beta-strand formation in peptides. The MAMBA scaffold is synthetically accessible and easily functionalized, thus demonstrating its potential to mimic diverse and chemically complex protein epitopes. The development of biomimetic synthetic regulators of complex protein interactions is of great clinical interest and provides new opportunities to study and rectify human disease states.



Beta-Strand Mimetic Conformation

The chemical structure and 2D NOESY assignments for a dimerized MAMBA peptidomimetic are shown (top); a crystal structure confirms the predicted hydrogen bonding pattern and conformation of the MAMBA dimer (bottom).

AEI 10

Incorporation of synthetic, toe-hold based gene circuits for the development of electrochemical sensors for rapid disease diagnostics

Sarah J. Smith¹, *sarahjane.smith@utoronto.ca*, **Shana O. Kelley¹**. (1) Pharmacy, University of Toronto, Toronto, Ontario, Canada (1) Univ Toronto Fac of Pharmacy, Toronto, Ontario, Canada

Techniques and diagnostic devices for use by non-specialists to detect disease states in low-resource areas are essential for combatting disease outbreaks. Importantly, for utilization outside of a laboratory setting, methods must be developed that are low-cost, and provide rapid and sensitive responses with little or no specialized equipment. Recent work has demonstrated the ability of toe-hold synthetic gene circuits to recognize specific proteins or nucleic acid sequences, including those associated with diseases such as Zika, activate gene expression, and produce a measurable protein signal. Optical detection has been used for these diagnostic systems, but here, we will detail the development of electrochemical methods which can provide a sensitive and economical alternative, and is more readily adapted for multiplexed detection. We utilize toe-hold gene circuits to develop platforms that can be rapidly adapted to sense an analyte of interest and produce outputs which can be readily detected electrochemically. For instance, in the presence of the desired analyte and subsequent “turn-on” of the gene circuit, a DNA restriction enzyme can be produced which modifies the surface of a DNA-bound electrode, changing the measured electrical current. Identification of multiple analytes with a single test can be performed by utilizing DNA sequences specific to different restriction enzyme outputs, enabling facile multiplexing without sacrificing sensitivity. Our progress in developing highly sensitive, low-cost, and readily adaptable diagnostic devices will be discussed.

AEI 11

Molecular Yoga: The juxtaposition of rational design and synthetic molecular evolution to create new, useful molecules

Gregory Wiedman, *gwiedman@jhu.edu*. Public Health Research Institute, Rutgers New Jersey Medical School, Newark, New Jersey, United States

Biomolecules: proteins, nucleic acids, lipids, are comprised of many static structures which build up in a hierarchical manner to form larger dynamic complexes. The classical view of dynamic structures is that they have evolved from facilitating non-specific interactions to specific interactions. There should exist enough space in the thermodynamic landscape of a molecule to allow it to access a number of different, discrete roles. My name is Dr. Gregory Wiedman and I am interested in taking structures that we typically think of as static and building them into dynamic structures. This includes protein alpha-helices, nucleotide quadruplexes, and lipid micelles. How exactly do transitions from random coil to alpha-helices enable amphipathic peptides to interact with cell membranes? Can we tune those transitions to improve peptide drugs? Is it possible for oligonucleotides with a multi-triplex or multi-quadruplex tertiary structure to have multiple induced-fit targets? Could fluctuations in nucleotide secondary structure be used for target-induced drug release? These are a few of the types of questions I hope to address in my laboratory. I see molecular design as an inherently iterative process that can draw from both rational design as well as synthetic evolution. My goal is to use tools from the areas of biochemistry, biophysics, and supramolecular chemistry to address these questions.

AEI 12

Derivatization of halopyridines for covalent enzyme inhibition

Alfred Tuley¹, *alfred.tuley@utexas.edu*, **Jake Swartzel²**, **Sean Patel²**, **Sarvnaz Sadrameli¹**, **Walter Fast¹**. (1) Pharmacy, The University of Texas at Austin, Austin, Texas, United States (2) Chemistry, The University of Texas at Austin, Austin, Texas, United States

Covalent enzyme inhibitors have garnered renewed interest in the past few years, largely stemming from the potency and selectivity advantages that covalent drugs have over non-covalent approaches. Recently, our group has discovered that fragment-sized 4-halopyridines can modify the active site cysteine of dimethylarginine dimethylaminohydrolase (DDAH-1), an enzyme critical for nitric oxide signaling. Follow-up studies have shown that halopyridines are largely inert towards free thiols, but can be modified in the specific microenvironment found in the DDAH-1 active site. Since this initial discovery, we have sought to derivatize halopyridines for a variety of applications, including attempts to enhance inhibitory properties and efforts to discover other targets for the halopyridine fragment. Herein, we will disclose the results of two key derivatization projects: 1) the synthesis and inhibitory constants of several amino acid-based halopyridines, and 2) the synthesis and proteomic impact of a structurally complex halopyridine probe. Undergraduate involvement in each project will be emphasized.

AEI 13

Rationally designed nanoscale catalysts for green transformations to form commodity chemicals

Hazim A. Al-Zubaidi, hazimabdulrazz.alzubaidi@wmich.edu, Sherine O. Obare. Chemistry, Western Michigan University, Kalamazoo, Michigan, United States

Well-defined and homogenous nanoscale monometallic and bimetallic catalysts composed of palladium, were rationally designed, synthesized, and characterized using new facile procedures. Transmission electron microscopy (TEM) and x-ray diffraction (XRD) were used for the characterization of the nanoparticle catalysts. The nanoparticles were immobilized on solid substrates and resulted in heterogeneous catalysts that were used for the conversion of model organic compounds into commodity chemicals. The effect of functional groups on the rate of the transformation of the organic compounds relative to the catalyst was investigated. The modified catalysts showed high selectivity and reactivity for the acetalization of selected aldehydes and ketones in the presence of alcohols. High yield of acetals and ketals were obtained at ambient pressure and temperature. The transformation intermediates and products were characterized using various spectroscopic techniques. The heterogeneous catalysts showed recyclability for eight catalytic cycles without significant loss in the selectivity and efficiency. The mechanisms for the catalytic reactions will be described.

Sulfur interactions with bimetallic Pd/Pt catalysts

Monique S. Wilburn^{1,2}, monique.wilburn1@yahoo.com, William S. Epling¹. (1) Chemical Engineering, University of Virginia, Charlottesville, Virginia, United States (2) Chemical and Biomolecular Engineering, University of Houston, Houston, Texas, United States

Having a high catalytic activity for hydrocarbon combustion, Pd-containing catalysts are commonly used in automotive-engine aftertreatment systems for emissions abatement. Since extended times on stream as well as high temperature, water, and trace sulfur exposure are associated with this application, these catalysts typically experience activity loss due to sintering and sulfur poisoning. Bimetallic Pd/Pt catalyst utilization has increased due to their improved activity and potential resistance to sintering. However, research shows that these bimetallic benefits were not observed in the presence of sulfur. Here, sulfur interactions with bimetallic Pd/Pt/Al₂O₃ catalysts were characterized.

Diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) and temperature-programmed desorption (TPD) studies show that SO₂ sorption characteristics depend on both precious metal crystallite particle size and Pd:Pt mole ratio. In general, the amount of SO₂ adsorbed and later desorbed during TPD decreased with increasing particle size or Pt content in the bimetallic Pd/Pt catalysts. Catalysts with a small particle size or high Pd content tended to have greater activity for oxidizing sulfur species at low temperatures and as a result formed more aluminum sulfate species. These sulfate species were stable and only decomposed at high temperatures. Large particle size or low Pd content catalysts tended to form more low-temperature decomposing and desorbing species, such as molecular SO₂ and aluminum surface sulfite.

To assess how sulfur exposure impacts catalytic activity, DRIFTS and CH₄ combustion studies were conducted with fresh and SO₂-treated Pt/Pd mono- and bimetallic catalysts. CO and SO₂ DRIFTS studies were used to identify sites impacted by SO₂ exposure and evaluate how the Pd:Pt mole ratio influences sulfur surface species formation. In an effort to recover CH₄ oxidation performance of SO₂-treated catalysts, temperature-programmed regeneration experiments were conducted in various gas environments. The findings show that for bimetallic catalysts with higher Pt content, the temperature-programmed regeneration methods had a greater negative impact on the catalytic activity than the sulfur exposure. Overall, this work provides evidence that sulfur interactions with bimetallic Pd/Pt catalysts vary with precious metal molar composition and over the life of the catalyst.

AEI 15

Maleic acid and aluminum chloride catalyzed conversion of glucose to 5-(Hydroxymethyl) furfural and levulinic acid in aqueous media

Ximing Zhang, zhan1290@purdue.edu. agricultural and biological engineering, Purdue University, West Lafayette, Indiana, United States

Maleic acid (MA) and AlCl_3 self-assemble into catalytic complexes ($\text{Al}-(\text{MA})_2-(\text{OH})_2(\text{aq})$) with improved selectivity for converting glucose to HMF, and levulinic acid. The calculated activation energy (E_a) of the MA-aluminum catalyzed glucose-to-fructose isomerization is significant lower for HCl and AlCl_3 alone. Furthermore, conversion of fructose to HMF is enhanced. The catalytic conversion of fructose to HMF by MA and AlCl_3 at 180°C is 1.7× faster with 3.3× higher selectivity when compared to HCl with AlCl_3 . Liquid ^{13}C NMR spectra results indicate that glucose undergoes a ring-opening process in aqueous solution when maleic acid is introduced, which we hypothesize facilitates the hydride shift in glucose for isomerization leading to enhanced rates and selectivity. Improved selectivity of glucose conversion to HMF and levulinic acid could improve the economics of producing these value-added chemicals for use in renewable, sustainable polymers.

AEI 16

Metal organic framework-modified graphene-based catalyst for oxygen reduction reaction

Shiqiang Zhuang, sz86@njit.edu, Bharath Babu Nunna, Eon Soo Lee. Mechanical Engineering, New Jersey Institute of Technology, Newark, New Jersey, United States

Nitrogen-doped graphene (N-G) is one of promising non-platinum group metal (non-PGM) catalysts for the oxygen reduction reaction (ORR). In this research, we investigated new N-G catalysts which are modified by the metal-organic framework (MOF), to enhance the electrochemical performance of N-G catalysts. The new MOF-modified N-G (N-G/MOF) catalysts with microporous structures are successfully synthesized by high energy nano wet ball milling methods with N-G and ZIF-8. The physical and chemical properties of new synthesized N-G/MOF catalysts are characterized several characterization methods such as XPS, XAS, SEM-EDS, TEM, XRD, BET and RRDE. The result shows that new microporous structures in NG/MOF catalysts were formed at 350 RPM which are totally different from structures of N-G and ZIF-8, and BET surface area is increased from 25 to 1103 (m²/gram). However, at 650 RPM the new microporous structures are suppressed to have no significant effect on the N-G structure. The ongoing research activities are trying to understand the synthesis reaction mechanism and to study the control of the synthesis mechanism through chemical and electrochemical characterizations of N-G/MOF catalysts. This research shows that the ZIF-8 could be a promising additive to modify physical, chemical, and catalytic performances of N-G catalysts. The successful accomplishment of the new N-G/MOF catalysts will provide the substantial way to the cost-effective and fuel-efficient energy conversion system.

AEI 17

Using LEGOs to help students understand kinetics and equilibrium concepts

Junyang Xian, xianjym@gmail.com, Daniel B. King. Drexel University, Philadelphia, Pennsylvania, United States

Kinetics and equilibrium concepts are difficult concepts for students to understand. The difficulty may come from the gap between their understanding of the phenomenon at the macroscopic level and their lack of understanding of the reactions at the microscopic level. It may be hard for students to imagine what is happening in a chemical reaction at the microscopic level since they can't actually see it. We used LEGOs to demonstrate a bimolecular reaction in entry-level chemistry classes and used this reaction to teach some kinetics and equilibrium concepts. Pre-test and post-test results were collected immediately before and after the LEGO activities to assess student learning. The experiment procedures were easy to learn and implement during class. In this presentation, results of nonparametric statistics tests that were performed on the pre- and post-tests will be reported. The results indicate the LEGO activities are able to help students understand chemical concepts that are directly related to the activities.

AEI 18

Nanoscale engineering for fundamental biophysical studies and biomedical applications

Swarnapali De Silva Indrasekara, swarnapaliindraserakara@gmail.com. Duke University, Durham, North Carolina, United States

Plasmonic nanomaterials, owing to their enhanced local electromagnetic field, are known to act as excellent sensors of their local environment through surface signal amplification. In particular, surface enhanced spectroscopies such as Raman scattering have shown promise even in single molecule detection. Therefore, there are much potential to understand biological processes and also to develop sensing technologies when plasmonic nanomaterials are properly integrated with Raman and optical spectroscopy techniques. To date, my contribution to this field of science has been two faceted; rational design and fabrication of optically active nanomaterials, and spectroscopic interrogation of processes occur at various nanoparticle interfaces for effective analytical and biomedical applications. My long-term career goal is to establish my own research group that utilizes nanoscale engineering and optical vibrational spectroscopy as tools to innovate new technologies to understand molecular as well as macro level processes significant in molecular biology, medicine, catalysis, and also to develop translational technologies for sustainable living and improved global health.

AEI 19

Potential of mean force for insertion of antimicrobial peptide melittin into a pore in mixed DOPC/DOPG lipid bilayer by molecular dynamics simulation

Yuan Lyu¹, lv10@purdue.edu, Ning Xiang¹, Xiao Zhu³, Ganesan Narsimhan². (1) Agricultural and Biological Engineering, Purdue University, West Lafayette, Indiana, United States (2) Dept of Agric Biological Eng, Purdue University, West Lafayette, Indiana, United States (3) Rosen Center for Advanced Computing , Purdue University, West Lafayette, Indiana, United States

Antimicrobial peptides (AMP) inactivate microorganisms by forming transmembrane pores in cell membrane through adsorption and aggregation. Energetics of addition of an AMP to a transmembrane pore is important for evaluation of its formation and growth. Such an information is essential for characterization of pore forming ability of peptides in cell membranes. This study quantifies the potential of mean force through molecular dynamics (MD) simulation for the addition of melittin, a naturally occurring AMP, into DOPC/DOPG mixed bilayer, a mimic of bacterial membrane, for different extents of insertion into either a bilayer or a pore consisting of three to six transmembrane peptides. The energy barrier for insertion of a melittin molecule into the bilayer was highest in the absence of transmembrane peptides and decreased for number of transmembrane peptides from three to six, eventually approaching zero. The decrease in free energy for complete insertion of peptide was found to be higher for larger pore size. Water channel formation occurred only for insertion into pores consisting of three or more transmembrane peptides with the radius of water channel being larger for larger number of transmembrane peptides. The structure of the pore was found to be paraboloid. Estimated free energy barrier for insertion of melittin into an ideal paraboloid pore accounting for different intermolecular interactions were consistent with MD simulation results. The results reported in this manuscript will be useful for the development of a model for nucleation of pores and a rational methodology for selection of synthetic antimicrobial peptides.

AEI 20

Self-assembly and applications of inverse opals

Katherine Phillips, *kphillips@fas.harvard.edu*. Research Laboratory for Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States

A number of optical, (electro)chemical, and sensing applications are enabled by defect-free inverted colloidal crystals, and the properties of these inverse opal structures are further expanded by controlling their composition. High-quality, crack-free inverse opals with minimal defects can be self-assembled using colloidal crystallization in the presence of a sol-gel precursor; in this poster, I will describe my work synthetically controlling the sol-gel chemistry of the matrix in order to control the shape and composition of inverse opals. With such fine control over the mesoscale structuration, inverse opals can be used as a model porous structure in a number of areas including electrocatalysis, catalysis, photochemistry, sensing, and heat transfer. I will also include my more recent work on one such application, namely the electrochemical reduction of CO₂.

AEI 21

Photoinduced single nanocrystal study of hybrid semiconducting nanomaterials

Prahlad K. Routh, *prahladkrouth@gmail.com*. Columbia University, New York, New York, United States

Nano-structured materials are the building blocks for next generation of opto-electronic devices as well as energy harvesting. Semiconducting nanocrystals have been the focus of study for solar energy harvesting and photodector based applications. Understanding of interfacial interactions between donor-acceptor systems have been the key to solve the challenges involved, especially in solution processable devices. The ultrafast dynamics of excitons among single nanocrystals has shown the potential to answer the inherent dynamic heterogeneities among donor-acceptor systems. In my research, model donor-acceptor systems have been studied using ultrafast photo excitation studies and competing mechanisms such as charge transfer and energy transfer has been investigated in polymer-nanocrystal hybrids and 0D-2D hybrids.

Metal nanoparticle decorated meso-graphene oxide composites as theranostics

Shruti Sharma³, shruti.sharma@stonybrook.edu, Lyufei Chen¹, Viet H. Pham⁴, James H. Dickerson⁴, Matthew A. Barish⁵, Rina Tannenbaum². (2) Materials Science and Engineering, Stony Brook University, Stony Brook, New York, United States (3) Materials Science and Chemical Engineering, Stony Brook University, Stony Brook, New York, United States (4) CFN, Brookhaven National Lab, Upton, New York, United States (5) Department of Radiology, Stony Brook University, Stony Brook, New York, United States

Carbon nanomaterials (CNMs) are emerging as materials of interest in biological applications such as, drug delivery, and tissue imaging, and particularly with respect to their selective toxicity in cancer tissues. Graphene oxide based CNMs (GO-CNMs) possess notable geometrical variants, such as flat sheets, tubes, scrolls and spheres, and form stable and easily-processed aqueous solutions. Further, the presence of oxygen containing functional groups in GO-CNMs provide potential locations for attachment of drugs, disease targeting functional groups as well as decoration with metal nanoparticles making them viable theranostics platforms. In this study, we decorated GO sheets with metal nanoparticles using methods reported elsewhere. Further, we developed a synthesis protocol for crumpled GO assemblies (GO roses) to produce metal nanoparticle decorated GO roses. Water-in-oil emulsions (W/O emulsion), used to fabricate the decorated GO roses, were obtained using a homogenizer. The aqueous phase of the W/O emulsion was rapidly removed from the system via evaporation due to emulsification in hot oil. The evaporation yielded spherical, crumpled meso-structures, ranging from sub-micron to several microns in size. We studied the morphology, chemical properties and theranostics capabilities of such composites with specific focus as potential cancer theranostics.

Design of crystalline heterosurfaces for direct nucleation of active pharmaceutical ingredients

Tharanga K. Wijethunga, *tharanga@mit.edu*, **Jelena Stojakovic**, **Fahimeh Baftizadeh**, **Allan S. Myerson**, **Bernhardt L. Trout**. Chemical Engineering, Massachusetts Institute of Technology, Quincy, Massachusetts, United States

Due to the inevitable presence of heterosurfaces and favorable energetics, most crystallizations are initiated by heterogeneous nucleation. However, the fundamental mechanistic understanding of heterogeneous nucleation is still deficient which hinders the design and use of heterosurfaces for direct control of crystallization. On the other hand, the use of functional, organic molecular, crystalline substrates is limited due to their inherently complex surfaces. In this study, we investigated and optimized nucleation of selected active pharmaceutical ingredients (APIs) using biocompatible, functional crystalline heterosurfaces. The selection criteria for the substrates were based on the compatible interacting functional groups between the substrate surface and the API of interest. Furthermore, we explored the possibility of polymorphic selection of the APIs with a rational selection of the substrates. The effectiveness of different substrates towards the enhancement of the API nucleation was measured using high-throughput *in situ* microscopy on a large number of crystallizations. Additionally, single crystal X-ray diffraction studies were conducted to identify the substrate crystal faces where API crystals were bound. The identified substrate faces were rich with possible interacting groups suggesting that when functional organic substrates belonging to low symmetry groups are utilized in crystallization processes, the crystallization outcome is directly affected by the intermolecular interactions between the substrate and the newly forming crystals. Our results indicate ways for fast and efficient selection of crystalline heterosurfaces for optimal nucleation of a given compound. Considering that, the main input for the selection is the compatible interacting sites on the heterosurface, we expect our results to be applicable to a wide range of crystallization processes.

AEI 24

Developing and applying computational approaches in early-stage drug discovery

Trent E. Balias, *talias@aol.com*. Pharmaceutical Chemistry, University of California, San Francisco, San Francisco, California, United States

In modern drug discovery, among the first steps is finding new lead molecules to modulate a protein drug target. My research focuses on developing and applying computational methods to aid in lead discovery. For example, I have implemented and tested new scoring terms for docking. Specifically, to understand the molecular recognition of a ligand and receptor, water energetics is very important. I have used all atom molecular dynamics (MD) simulations, and grid-based inhomogeneous solvation theory (GIST) to account for receptor water displacement in docking discovery campaigns. I have also used MD and Free energy methods for understanding binding energies and drug resistance. In my future research, I will use docking, MD, free energy calculations, and GIST to aid in the discovery of new molecules that circumvent drug resistance in cancers and infectious diseases.

AEI 25

Power of exact using conditions to develop density functionals

Duminda S. Ranasinghe, *dranasinghe@chem.ufl.edu*, **Johannes T. Margraf**, **Rodney J. Bartlett**. Department of Chemistry, University of Florida, Gainesville, Florida, United States

A correlated orbital theory (COT) has an effective one-particle operator which include electron correlation. Kohn-Sham density functional theory (KS-DFT), can be considered as a COT. One of the conditions that COT should satisfy is that orbital eigenvalues approximate the exact principal ionization potentials for occupied orbital in a molecule. Under GKS-DFT formalism, the IP condition is a consequence of adiabatic TDDFT and beyond being an accurate approach for excitation energies. When an electron is excited into the continuum, all the KS ground state orbital energies should be good approximations to IP's. To satisfy the COT IP condition for m^{th} orbital, $-IP_m = \epsilon_m = \langle \phi_m | H + J - K + \Sigma_{cc} | \phi_m \rangle \approx \langle \phi_m | H + J + V_{xc} | \phi_m \rangle$ demands that V_{xc} be an accurate approximation to the non-local, $-K + \Sigma_{cc}$, where H , J , K , Σ_{cc} , and V_{xc} stands for one-electron Hamiltonian, coulomb integral, exchange integral, self-energy, and coulomb and exchange potential respectively. Guided by this principle minimally parameterized QTP functionals were constructed. These QTP functional showed less self-interaction error, correct bond dissociating curves, correct long-range behavior for charge transfer complex, and competitive thermochemical accuracy when compare to similar functionals. QTP00 functional showed excellent results for core excitations and QTP01functional also showed the accurate prediction of valence and Rydberg excitation. QTP02 functional is based on ω B97 formalism and an improvement upon QTP00 and QTP01.

Deep learning vs Zika virus: At the crossroads of computational chemistry, systems biology, data mining and computer science

Natalia Sizachenko, *sizachenko@icnanotox.org*. Interdisciplinary Center for Nanotoxicity, Jackson State University, Jackson, Mississippi, United States

Mosquito-borne viruses of Flaviviridae virus family (West Nile virus, Zika virus, Yellow fever virus) are dangerous for human. For the last couple of years, enormous amounts of money are spent in both academia and industry on the investigation of mosquito-borne viruses, especially Zika virus. Usually, antiviral drugs, as well as treatment with interferons, do not have a positive effect on patients. The aim of proposed project is deep computational search of suitable drugs. Activation of non-structural proteins NS1, NS2A, NS3 and NS5 inside of mosquito-borne viruses is necessary for viral replication. At the same time, structural envelop protein is involved in entry of viral particles into the cell. Hence, inhibition of these proteins could neutralize the virus. As genome and biochemistry of mosquito-borne viruses is similar, the main challenge is to identify lead compounds which could simultaneously inhibit all three viruses. Combination of learning techniques was applied to find the best candidate drug.

Pushing nonlinear spectroscopy to its limit: Theoretical upper bounds for second harmonic generation in molecules and materials

Liang Zheng Tan², *liangtan@sas.upenn.edu*, **Andrew M. Rappe**¹. (1) University of Pennsylvania, Philadelphia, Pennsylvania, United States (2) Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania, United States

Nonlinear optical response is immensely important in the spectroscopy of molecules and materials, and includes a diverse set of phenomena such as second harmonic generation (SHG), two photon absorption, sum frequency generation, and excited state absorption, among others. In practical applications of SHG, it is often of interest to maximize the magnitude of nonlinear response, in order to increase the efficiency of the frequency conversion devices. The choice of materials in these applications is usually driven by trial and error, with limited theoretical guidance. Despite decades of research into nonlinear response theory, and the occasional discovery of materials with large nonlinear responses, there has been no systematic investigation into the maximum amount of SHG attainable in real materials.

In this theoretical work, I present an upper bound for the SHG response of any molecule, regardless of its size or complexity. Using the shift vector formulation of SHG, I derive an analytic expression for the upper bound, showing that the frequency-integrated SHG response tensor must take values less than a certain threshold. This framework is then generalized to extended systems such as crystals, where it is shown that the upper limit of SHG is controlled by the band gap, band width, and covalency of the crystal. As a proof of principle, I calculate the SHG response tensors of a wide variety of materials and molecules, using a perturbation theory approach based on density functional theory (DFT), finding all calculations to be consistent with the theoretical upper bound. These first-principle calculations indicate that most known materials do not yet saturate the upper bound, and it is likely that new large SHG materials will be discovered by future materials research.

Computational study of ketoheptylperoxy radical atmospheric decomposition and combustion

Alexander C. Davis, *caffeine_chemist@hotmail.com*. Chemistry, Franklin and Marshall College, Lancaster, Pennsylvania, United States

With growing concern about both the finite nature of traditional petroleum based fuels and their relation to climate change there is a clear need to increase our understanding of how these fuels, and potential new biofuels, react under combustion and atmospheric conditions. Both processes involve the oxidation of hydrocarbons, with sequential steps leading to increasingly oxidized species. The study reported here uses n-ketoheptyl-m-peroxy radicals, where n ranges from 1-4 and m ranges from 1-7, as a model system for studying the unimolecular decomposition of these oxygenated hydrocarbons. All geometry optimizations and frequency calculations are carried out using the Gaussian 09 suite of programs. Final energy calculations were conducted using the CBS-QB3, G3 and G4 composite methods, which were selected for their reported accuracies of ~ 4 kJ mol⁻¹. Rate parameters were determined using ChemRate, which includes Eckart tunneling and Pitzer and Gwinn 1D hindered rotor treatments. Initial results suggest that the location of the ketone group within the ring structure of transition state structures may increase the rate of H-migration reactions and that when the peroxy group is beta to the ketone, C-C bond scission is the dominant pathway under both atmospheric and combustion conditions.

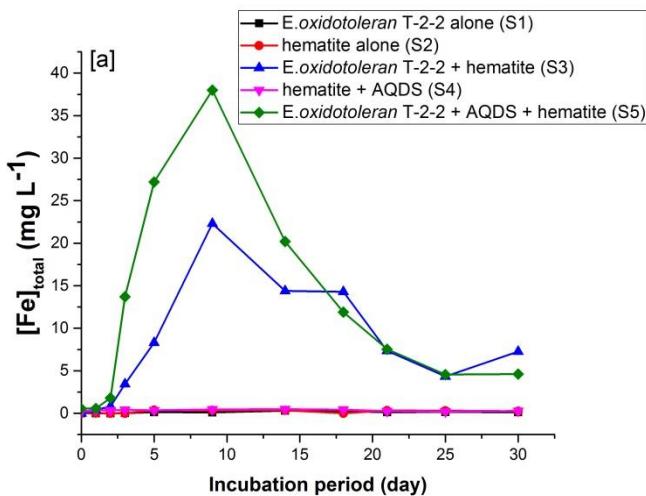
Microbial effect of iron from hematite into seawater mediated via anthraquinone-2,7-disulfonate

Apichaya Aneksampant, apichaya.aneksampant@gmail.com. Engineering, Hokkaido University, Sapporo, Hokkaido, Japan

The restoration of seaweed beds has been developed using a fertilizer for supplying dissolved Fe to barren coasts. The fertilizer is composed of iron oxides as a source of Fe and compost as humic substance (HS) source, which can serve as a chelator to stabilize the dissolved Fe in oxic seawater. However, elution mechanisms of Fe from iron oxide have not sufficiently elucidated. Fujisawa et al. suggests that the fertilized HSs in barren coast are decomposed via microbial processes. This may be related to the elution of Fe from iron oxide. In the present study, microorganisms from incubated fertilizer in barren coast were isolated and inoculated to artificial seawater that contained hematite as a model of iron oxide. In addition, the effect of anthraquinone-2,7-disulfonate (AQDS) as a model of HS on the Fe elution was investigated. The fertilizer was incubated in a water tank at the Mashike coast (Hokkaido, Japan).

E.oxidotolerans(T-2-2) was isolated. Test for Fe elution was performed by the inoculation of T-2-2 in postgate B medium for 1 month for (i)T-2-2 alone, (ii)hematite alone, (iii) (i)+hematite, (iv) (i)+AQDS, (v) (iii)+AQDS and (vi) (ii), hematite and AQDS were included 4 gL⁻¹ and 2 gL⁻¹, respectively. The eluted iron was analyzed by ICP-AES.

Figure 1 shows the elution kinetics of Fe from hematite. During the incubation period, Fe elution was reached the highest level after 9 days of incubation and then decreased to stabilize for seawater, contained both T-2-2 and AQDS. For control and uninoculated culture, a trace amount of Fe were eluted during 30 days, suggesting that Fe elution into seawater can be due to microbial activities. Thus AQDS can enhance the microbial elution of Fe.



Predicting solvent-water partitioning of charged organic species using quantum-chemically estimated Abraham pp-LFER solute parameters

Craig Davis¹, davi3148@umn.edu, Dominic M. Di Toro². (1) Civil, Environmental, & Geoengineering, University of Minnesota, Minneapolis, Minnesota, United States (2) Civil & Environmental Engineering, University of Delaware, Newark, Delaware, United States

Methods for obtaining accurate predictions of solvent-water partitioning for neutral organic chemicals (e.g., octanol-water partition coefficients) are well established. However, methods that provide comparable accuracy are not available for predicting the solvent-water partitioning of ionic species. Recent work by Franco et al. has demonstrated that for a subset of the 117,000 organic chemicals registered in the European REACH database, approximately 33% have been shown to be “significantly ionized” at environmentally relevant pH values (pH ~ 7.0).

Consequently, 1/3 of the chemical database lacks a predictive model for accurately determining the partitioning, and ultimately the fate and transport, of these chemicals in the environment. This paper outlines a method of predicting solvent-water partition coefficients for ionic species using Abraham pp-LFER solute descriptors estimated from quantum chemistry. For a suite of carboxylic acid anions, solvent-water partition coefficients for 4 solvent-water systems: acetonitrile-, acetone-, methanol-, and dimethylsulfoxide-water (computed from experimental ionization constants in the solvents and water) were predicted with root mean square (RMS) errors of 0.475, 0.512, 0.460, and 0.393, respectively (n = 44, 48, 47, and 41). For a larger set of substituted quaternary amine cations (n = 217), experimentally determined octanol-water partition coefficients were predicted with an RMS error of 1.16.

Predictions made using the quantum-chemically estimated Abraham parameters (QCAPs) were shown to provide improved accuracy in predicting solvent-water partition coefficients, compared to predictions of solvent-water partition coefficients, made using existing Absolv-estimated Abraham solute descriptors derived from the neutral species. For partitioning of anionic solutes in the four organic solvent-water systems, the overall RMS errors were 0.740 and 0.462 for the Absolv and QCAP methods, respectively. For cations partitioning into octanol the overall RMS errors were 0.997 and 1.16, respectively.

The QCAP method demonstrated improved accuracy over directly-calculated ab initio quantum chemical partition coefficients at comparable levels of theory (M062X/6-31++G**) for both anions partitioning into the 4 organic solvents (RMSE = 0.462 vs. 2.48 for QCAP-predicted vs. direct QC computed, respectively) and cations partitioning into octanol (RMSE = 1.16 vs. 2.82 for QCAP-predicted vs. direct QC computed, respectively).

Elucidating mechanisms of toxicity of nanoparticles exposed to various environmental factors

Niluka M. Dissanayake, nilukamadhumi.m.dissanayake@wmich.edu, Sherine O. Obare.

Chemistry, Western Michigan University, Kalamazoo, Michigan, United States

In recent years, there has been an increased interest in the design and use of nanoscale materials for various technological applications and in consumer products. In particular, iron oxide nanoparticles (IONPs) with nanoscale dimensions have shown favorable magnetic, catalytic, biomedical, and electronic applications. The increased manufacture and use of nanoparticles in consumer products as well as industrial processes is expected to lead to their unintentional release into the environment. The impact of IONPs and other nanoparticles on the environment and on biological species is not well understood, but remains a concern due to the increased chemical reactivity of nanoparticles relative to their bulk counterparts. The studies focus on understanding factors that need to be considered when various nanoparticles including IONPs are placed in the environment. We show the influence of nanoparticles on microorganisms, particularly on those required for bioremediation. The results shed light on the transformations nanoparticles undergo in the environment, the potential mutagenic effect on biological cells, and the impact on the ecosystem.

Preparation of chloraminated concentrated drinking water for disinfection by-product mixtures research

Alison R. Kennicutt, *akennicutt@gmail.com*, **Paul Rossman**, **Jonathan G. Pressman**, **David Wahman**. U.S. Environmental Protection Agency, Cincinnati, Ohio, United States

Complex mixtures of disinfection by-products (DBPs) are formed when the disinfectant oxidizes constituents (e.g., natural organic matter (NOM) and organic pollutants) present in the source water. Since 1974, over 600 DBPs have been identified in drinking water, yet a large portion of the total organic halogens formed remain unidentified. Concerns for public health continue to drive DBP research as increased exposure has been associated with carcinogenic and/or endocrine disrupting properties. Toxicological evaluation of whole DBP mixtures, including the unidentified DBPs, allows a more accurate accounting of the magnitude of health effects. This work evaluates chloramination by preformed monochloramines and chloramination that is preceded by various free chlorine contact periods, which is a continuation required because of the complexity of chemical reactions with respect to chloramines, bromide, iodide, and the resulting DBPs formed. The primary objective of this research was to create DBPs that are representative of chloraminated water systems while producing concentrated whole mixtures of DBPs that scale with total organic carbon (TOC) concentration for future DBP toxicology studies.

Ohio River water was collected post-ultrafiltration (UF1X) and as reverse osmosis concentrate that had been concentrated 142-times the UF1X TOC concentration. A portion of the concentrate was freeze-dried to produce a solid NOM that was reconstituted at defined TOC concentrations, representing 1-times, 142-times, and 500-times the UF1X TOC. The concentrate was also diluted down to an equivalent 1X TOC. Bromide (1X=115 µg/L) and iodide (1X=11.5 µg/L) were added to a pH 8 phosphate buffered waters. All samples were analyzed for 57 individual DBPs.

Chloramination was conducted by dosing 1X waters with 2.5 mg/L of preformed monochloramine or 2.5 mg/L free chlorine followed by ammonia (4.75:1 chlorine to ammonia-nitrogen ratio). For 1X waters, a 3-minute and a 20-minute free chlorine contact time respectively corresponded to 80% and 100% bromide oxidation and 65% and 100% iodide oxidation. Initial experiments and a free chlorine/chloramine kinetic model were used to establish initial dosing concentrations and reaction times required to scale 1X to 142X and 500X. For DBP formation, comparisons will be presented for the (1) various chloramine dosing scenarios, (2) impact of concentration, (3) and impact of NOM processing (e.g., freeze-drying and reconstitution).

Investigating sources, fates, and biological effects of emerging organic contaminants using innovative passive monitoring tools and integrative measures of toxicity

Carrie A. McDonough^{2,1}, carriemc@my.uri.edu, Christopher P. Higgins¹, Rainer Lohmann². (1) CEE Dept., Colorado School of Mines, Golden, Colorado, United States (2) University of Rhode Island, Narragansett, Rhode Island, United States

My overarching goal as an independent researcher is to lead an ambitious, interdisciplinary research program at the intersection of environmental chemistry and molecular toxicology, with a focus on contaminant source fingerprinting, biomarker identification, and socioeconomic determinants of human pollutant exposure and health outcomes. In my postdoctoral work at CSM, I am currently investigating the toxicodynamics and biological effects of per- and polyfluoroalkyl substrances (PFASs) and their metabolites in the body to better understand how chronic exposure to complex mixtures of PFASs in drinking water affects human health.

My Ph.D. work at URI, which has led to three first-author publications to date, was an ambitious, interdisciplinary project that contributed to scientific understanding of spatial distributions, environmental transport, and effects of organic contaminants, and furthered development of innovative monitoring tools for organic contaminants. Key findings from this work include calculation of the first air-water diffusive exchange rates for organic contaminants in the region using co-deployed air and water samplers, showing that the lakes acted as secondary sources of synthetic fragrances and remained a sink for phased-out brominated flame retardants. This work also demonstrated that the influence of nearby population centers on spatial distributions of gaseous organic contaminants depends on compound vapor pressure, and made use of advanced spatial data analysis techniques to interpolate dissolved flame retardant concentrations over the entire Great Lakes region, offering the first predictions of dissolved flame retardant concentrations across the lakes. I also spearheaded an interdisciplinary collaborative study using *in vitro* aryl hydrocarbon receptor-mediated bioassays to measure integrated effects of environmentally relevant mixtures of air pollutants isolated from passive air samplers from the Great Lakes, which showed that <30% of observed biological potency could be explained by regularly monitored PAHs. Along with work on the Great Lakes, I investigated global fate and long-range transport of currently used organophosphate flame retardants using passive water samplers deployed in the North Atlantic and Canadian Arctic. Results suggest concentrations are much greater than those of other flame retardants, highlighting the organophosphate FRs as an important group of emerging contaminants with unknown impacts on remote environments.

Coupled microbial electrolysis cell-forward osmosis system for sustainable wastewater treatment and resource recovery

MOHAN QIN, *mohanq@vt.edu*, Zhen He. Civil and Environmental Engineering, Virginia Tech, Blacksburg, Virginia, United States

Wastewater is treated for contaminant removals and bioenergy recovery; however, the valuable resources in wastewater, such as nutrients and water, have not been well recovered for reuse. Extracting water from wastewater can be accomplished by using membrane processes, but the energy in organic compounds in the remaining concentrates was not recovered. Nitrogen recovery from wastewater requires energy-intensive processes such as struvite formation. Herein, a new concept of a microbial electrolysis cell (MEC)-forward osmosis (FO)-coupled system was proposed for wastewater treatment and recovery of both clean water and nitrogen with low energy consumption. In MEC, the organic compounds were degraded while the generated electricity facilitated the recovery of ammonium nitrogen which was collected to prepare ammonium bicarbonate. In FO, the generated ammonium bicarbonate was used as draw solutes to extract clean water from the MEC anode effluent. The feed concentrates from FO could return to MEC anode for further recovery. The feasibility of the above concept was investigated in this study. The recovered ammonium from MEC could reach a concentration of 0.86 mol L^{-1} , and with this draw solution, $50.1 \pm 1.7 \%$ of the MEC anode effluent could be extracted in FO. The results have successfully demonstrated the feasibility of coupling an ammonia-recovering MEC with FO for treating high-strength wastewater and recovering valuable resources with low energy consumption.

Removal of trace organic contaminants and estrogenic activity in six full-scale integrated fixed-film activated sludge (IFAS) wastewater treatment plants

Michael Shreve, mjs697@psu.edu, Rachel Brennan. Penn State, State College, Pennsylvania, United States

Pharmaceuticals and personal care products (PPCPs), human hormones, pesticides, surfactants, and other anthropogenic chemicals are routinely detected in domestic wastewater, often at low concentrations (ng/l - μ g/l). Many of these trace organic contaminants (TrOCs) pass through conventional treatment systems (e.g. activated sludge, AS) and are discharged with treated effluent into surface waters, posing risks for aquatic ecosystems and downstream potable water intakes. The integrated fixed-film activated sludge (IFAS) process provides a means of upgrading existing conventional activated sludge wastewater treatment plants (CAS-WWTPs) by adding free-floating plastic media which provide surface area for biofilm growth in the otherwise suspended growth reactors. The increase in overall biomass increases treatment capacity and the biofilm provides a niche for slow-growing microbes, such as ammonia oxidizing bacteria, which improve nitrogen removal. While IFAS upgrades are typically implemented to increase a WWTP's capacity to remove easily degradable organic compounds and nutrients, several bench- and pilot-scale studies suggest that TrOC removal may also be improved. However, no investigation of TrOC removal in full-scale IFAS-WWTPs has been published. In this study, six full-scale IFAS-WWTPs were surveyed to quantify the removal of TrOCs and associated hormone disrupting activity. The microbial diversity of both suspended and biofilm communities was also investigated. For each IFAS-WWTP, 24 h composite samples of secondary influent and effluent were analyzed for total suspended solids (TSS), chemical oxygen demand (COD), ammonia, estrogenic activity, and 98 TrOCs. DNA was extracted from duplicate grab samples of AS and IFAS media, PCR amplified to target fungi (ITS2) and bacteria/archaea (V4, 16s), then submitted for high-throughput sequencing on an Illumina MiSeq. All IFAS-WWTPs efficiently removed TSS, COD, and ammonia. Thirty-four of the targeted TrOCs were not detected in any WWTP, while twenty-seven showed consistently high removal ($\geq 99\%$ average). The remaining TrOCs had highly variable removal rates, but qualitative assessment shows higher removals for acesulfame-k, atenolol, diclofenac, and TCPP, when compared to values found in the literature for CAS-WWTPs. Removal of estrogenic activity was generally greater than 80%, and effluent values ranged from below detection to 19.4 ng/L estradiol equivalents. Microbial diversity analyses remain in progress.

Quantitative SERS enabled by surface plasmon enhanced elastic scattering

Haoran Wei², haoranw@vt.edu, Weinan Leng¹, Peter J. Vikesland¹. (1) Virginia Tech, Blacksburg, Virginia, United States (2) Civil and Environmental Engineering, Virginia Tech, Blacksburg, Virginia, United States

Surface-enhanced Raman spectroscopy (SERS) has long been proposed as an ultrasensitive analysis method with single molecule level sensitivity, minimal need for sample pretreatment, rapid detection time, and potential for on-site deployment. However, in spite of the large volume of research conducted to develop SERS substrates and optimize the technique, the poor reproducibility of the SERS signal makes it a challenge to achieve reliable quantitative SERS analysis. Herein, we demonstrate a novel approach for quantitative SERS analysis that exploits surface plasmon enhanced Rayleigh scattering signals as internal standards for SERS signal normalization. Our measurements show that the intensity of the surface plasmon enhanced elastic scattering signal of a low-wavenumber pseudo-band (ν_e) scales linearly with the integrated SERS "hot-spot" signal strength. This pseudo-band can be used as an internal standard to calibrate SERS "hot spot" variations and minimize the inherent signal heterogeneity of a given SERS substrate. Internal standards based on surface plasmon enhanced elastic scattering signals are truly intrinsic to the plasmonic nanostructures and provide new features that significantly improve quantitative SERS analysis: (1) ultimate photo-stability (i.e., not photo-bleachable); (2) minimal spectral interference with analyte Raman signals; (3) no spatial competition with analyte molecules for SERS "hot spots"; and (4) reduced SERS substrate preparation costs by avoiding the incorporation of extrinsic reference probe molecules.

Water-solute permselectivity limits of biomimetic desalination membranes

Jay R. Werber, jay.werber@gmail.com, Menachem Elimelech. Chemical and Environmental Engineering, Yale University, New Haven, Connecticut, United States

Membrane-based desalination is increasingly applied to alleviate water scarcity through the purification of nontraditional water sources, such as seawater, brackish groundwater, and municipal wastewater. Due to fundamental material limitations, the performance of the industry standard thin-film composite (TFC) membranes has largely plateaued. As such, there has been highly active research in exploiting biological water channels, such as the membrane protein aquaporin, or synthetically-designed water channels to produce “next-generation” desalination membranes. Most of these design strategies would incorporate the channels within an amphiphilic lipid or block copolymer bilayer to form the membrane selective layer. As most of the membrane surface area would comprise just the bilayer, the permeability characteristics of the bilayer plays a crucial role in determining the overall water/solute permselectivity of the resulting membrane. In this study, solution-based analytical methods are used to measure the permeability of water and solutes with varying size and solubility characteristics through lipid and block copolymer bilayers. Results are combined with published single-channel permeabilities to yield the permeability and selectivity limits of defect-free biomimetic membranes. Comparison with the performance of a commercial TFC membrane shows that biomimetic desalination membranes may be advantageous for some desalination applications, but disadvantageous for others.

Alkylation of benzene with ethylene in the presence of zeolite catalyst: Mathematical modelling of reactor

Elena Khlebnikova¹, elena.khle@gmail.com, Elena Ivashkina¹, Irena Dolganova¹, Igor Dolganov¹, Stanislav Koshkin². (1) Department of Fuel Engineering and Chemical Cybernetics, Tomsk Polytechnic University, Tomsk, Russian Federation (2) LLC NIOST, Tomsk, Russian Federation

This paper presents the analysis results of operation of the industrial alkylation reactor. Based on the process chemism, the list of possible reactions by calculating the Gibbs energy with the use of quantum chemistry methods was compiled.

Thermodynamic values for chemical reactions were calculated using quantum chemical methods and confirmed the targeted alkylation of benzene with ethylene, the transalkylation of polyethylbenzene; cracking side reactions and alkenes cyclization, cycloparaffins cracking, conjugate hydrogenation, diphenylethane formation, condensation and oligomerization.

Based on these results, as well as on the material balance of the process, which is given in the regulation of production, the key substances involved in the conversion or resulting from their occurrence were identified (Table 1). Among them there are fractions: combined group of alkanes and alkenes having from 1 to 5 carbon atoms; cycloalkanes C6 (cyclo-A) mainly consisting of methylcyclopentane (M cycloP) and cyclohexane (cycloH); cycloalkanes C7 consisting mainly of methylcyclohexane (M cyclo-H) and dimethylcyclopentane (diM cycloP); heavy components of 1,2 - diphenylethane (diPhE) and polyalkylbenzenes (PABs) - products of further ethylene alkylation and alkylation products with long chain (C5-C7) alkenes; resinification and dehydrocyclization products. Also some substances or their isomeric mixtures were identified: ethylbenzene (EB), benzene (B), paraffin (P), toluene (T), diethylbenzenes (diEB), triethylbenzene (triEB), butylbenzene (BB).

Taking into account the list of occurring reactions and the list of pseudo components mathematical model of alkylation according to plug flow reactor model was developed. Estimated error of this model does not exceed 10%, which allows using it in order to optimize the modes of industrial alkylation process.

The list of reactions and kinetic equations	The rate of formation and consumption of individual components
<ol style="list-style-type: none"> $E + B \leftrightarrow EB$ $r_1 = k_1 C(E)C(B) - k_{-1} C(EB)$ $EB + E \leftrightarrow diEB$ $r_2 = k_2 C(EB)C(E) - k_{-2} C(diEB)$ $diEB + E \leftrightarrow triEB$ $r_3 = k_3 C(diEB)C(E) - k_{-3} C(triEB)$ $diEB + B \leftrightarrow 2EB$ $r_4 = k_4 C(diEB)C(B) - k_{-4} C(EB)^2$ $EB + B \leftrightarrow diPhE + 0.038P$ $r_5 = k_5 C(EB)C(B) - k_{-5} C(diPhE)C(P)$ $triEB + E \leftrightarrow T$ $r_6 = k_6 C(triEB)C(E) - k_{-6} C(T)$ $diEB \rightarrow 0.705T$ $r_7 = k_7 C(diEB)$ $P + B \leftrightarrow 0.689T$ $r_{8a} = k_{8a} C(P)C(B) - k_{-8a} C(T)$ $P + EB \leftrightarrow 0.837T$ $r_{8b} = k_{8b} C(P)C(EB) - k_{-8b} C(T)$ $P + diEB \leftrightarrow 0.984T$ $r_{8c} = k_{8c} C(P)C(diEB) - k_{-8c} C(T)$ $P + triEB \leftrightarrow 1.132T$ $r_{8d} = k_{8d} C(P)C(triEB) - k_{-8d} C(T)$ $cycloH \leftrightarrow 1.585P$ $r_9 = k_9 C(cycloH) - k_{-9} C(P)$ $M cycloH \leftrightarrow 1.849P$ $r_{10} = k_{10} C(M cycloH) - k_{-10} C(P)$ $BB \leftrightarrow B + 1.056P$ $r_{11} = k_{11} C(BB) - k_{-11} C(B)C(P)$ $BB \leftrightarrow EB + E$ $r_{12} = k_{12} C(BB)$ $2E \leftrightarrow 1.056P$ $r_{13} = k_{13} C(E)^2$ 	$ \begin{aligned} r(E) &= -r_1 - r_2 - r_3 - r_6 + r_{12} - 2 \cdot r_{13} \\ r(B) &= -r_1 - r_4 - r_5 - r_{8a} + r_{11} \\ r(EB) &= r_1 - r_2 + 2 \cdot r_4 - r_5 - r_{8b} + r_{12} \\ r(diEB) &= r_2 - r_3 - r_4 - r_7 - r_{8c} \\ r(triEB) &= r_3 - r_6 - r_{8d} \\ r(diPhE) &= r_5 \\ r(BB) &= -r_{11} - r_{12} \\ r(cycloH) &= -r_9 \\ r(M cycloH) &= -r_{10} \\ r(P) &= 0.038r_5 - r_{8a} - r_{8b} - r_{8c} - r_{8d} \\ &\quad + 1.585r_9 + 1.849r_{10} \\ &\quad + 1.056r_{11} + 1.056r_{13} \\ r(T) &= r_6 + 0.705r_7 + 0.689r_{8a} \\ &\quad + 0.837r_{8b} + 0.984r_{8c} \\ &\quad + 1.132r_{8d} \end{aligned} $

Hydroxylamine oxidoreductase activities and bacterial ammonia oxidation pathways

Jonathan D. Caranto, jonathan.caranto@gmail.com. Chemistry and Chemical Biology, Cornell University, Ithaca, New York, United States

Substantial amounts of nitric oxide (NO) and nitrous oxide (N₂O) are released as by-products of ammonia (NH₃) oxidation to nitrite (NO₂⁻) mediated by NH₃-oxidizing bacteria (AOB). N₂O has a global warming potential ca. 300 times greater than that of carbon dioxide, whereas NO contributes to ground-level ozone and acid rain. These emissions can be exacerbated by fertilization, which is necessary for large-scale agriculture. Elucidation of biological NH₃-oxidation pathways could lead to strategies for limiting these NO and N₂O emissions.

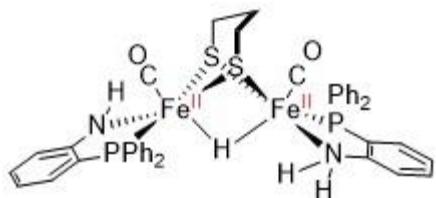
For the currently accepted model of AOB metabolism, NH₃ is oxidized to NO₂⁻ via a single obligate intermediate, hydroxylamine (NH₂OH). Within this model, the enzyme hydroxylamine oxidoreductase (HAO) catalyzes the 4-electron oxidation of NH₂OH to NO₂⁻. NO is proposed to result from the incomplete oxidation of NH₂OH by HAO under low O₂ concentration; reduction of this NO by nitric oxide reductases (NORs) results in N₂O. The HAO active site is termed a P460 cofactor, which exhibits a unique tyrosine crosslink to a c-type heme. A second, unrelated enzyme called cytochrome (cyt) P460 exhibits a similar active site, in which lysine, not tyrosine, crosslinks with the heme. Despite this difference, cyt P460 was shown to exhibit similar NH₂OH oxidase activity to form NO₂⁻.

We recently reevaluated the cyt P460 activity and showed that it oxidized NH₂OH to N₂O. We proposed NO₂⁻ to be a *non-enzymatic product* resulting from the reaction of O₂ with NO that dissociates from an intermediate ferric-nitrosyl species. These results inspired us to reevaluate NO₂⁻ as an enzymatic product of HAO. This presentation will provide evidence that HAO oxidizes NH₂OH to NO, not NO₂⁻. Thus, NO is an obligate intermediate of AOB metabolism, acting as a branch point for NO₂⁻ and N₂O production and NO emission. These results also imply a third, unidentified, enzymatic nitrification step that oxidizes NO to NO₂⁻.

Diiron complexes with new proton-relay ligand platforms

Michaela R. Carlson³, mcarlson42@me.com, **Timothy W. Chapp**¹, **Ryan Gilbert-Wilson**³, **Joyee Mitra**³, **Thomas B. Rauchfuss**². (1) Chemistry, Allegheny College, Meadville, Pennsylvania, United States (2) A131CSSL Box 60-6, University of Illinois, Urbana, Illinois, United States (3) Chemistry, University of Illinois at Urbana-Champaign, Urbana, Illinois, United States

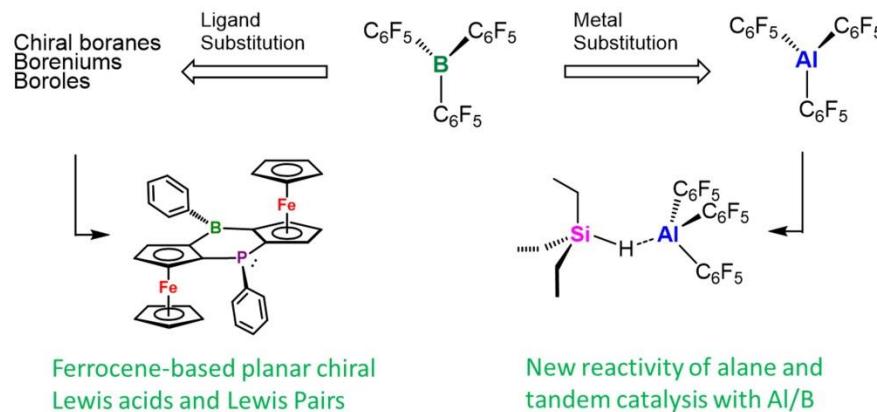
We will report two new proton-relay ligand platforms, diphenylphosphinoaniline and diphenylphosphine oxide. An amido neutral μ -hydride, $[\text{HFe}_2(\text{pdt})(\text{CO})_2(\text{PNH})(\text{PNH}_2)]$, was afforded via reaction of $\text{Fe}_2(\text{pdt})(\text{CO})_6$ with two equiv of diphenylphosphinoaniline (PNH_2). We will describe the proton exchange behavior of this amido-amine as well as its conversion to the diamine $[\text{HFe}_2(\text{pdt})(\text{CO})_2(\text{PNH}_2)_2]^+$ and the diamide $[\text{HFe}_2(\text{pdt})(\text{CO})_2(\text{PNH})_2]^{-1}$. We will also describe another μ -hydride species, confirmed via NMR spectroscopy, with the nominal formula $\text{Fe}_2(\text{edt})(\text{CO})_3(\text{HOPPh}_2)_3$. As in the $\text{Fe}_2\text{-PNH}_2$ case, these Fe_2 -phosphinous acid complexes display rich acid-base behavior.



Planar chiral, redox active and strongly Lewis acidic organoboranes and organoalanes: Isolation, structural characterization and diverse catalysis

Jiawei Chen², cjiaw@hotmail.com, Frieder Jaekle³, Eugene Y. Chen¹, Jack R. Norton². (1) Colorado State University, Fort Collins, Colorado, United States (2) Columbia Univ, New York, New York, United States (3) Rutgers Univ, Newark, New Jersey, United States

$B(C_6F_5)_3$, owing to its remarkable acidity and stability, has been widely used as a (co)catalyst in a variety of areas such as Lewis acid-mediated small molecule transformations, frustrated Lewis pairs chemistry, and polymer synthesis. Recent efforts have been focused on Lewis acidity enhancement, new reactivity and asymmetric catalysis development. Replacement of the boron center with its heavier analog Al or decoration of its peripheral ligand sphere allows us to obtain a series of novel Lewis acids and subsequently explore the unique properties and reactivities that are not accessible with $B(C_6F_5)_3$ (Scheme 1). For example, we found that $Al(C_6F_5)_3$ is capable of forming an elusive and stable alane-silane adduct, which is believed to involve in four different type of catalytic transformations including polymerization, hydrodefluorination, hydrosilylation and silane redistribution. The combination of $B(C_6F_5)_3$ and $Al(C_6F_5)_3$ also enables the activation of greenhouse gas CO_2 and selective reduction to methane (Figure 1). In addition, we demonstrated the incorporation of 1,2-disubstituted ferrocene frameworks onto Lewis acidic boron can serve as an effective strategy for the construction of planar chiral yet redox-active Lewis acids/Lewis pairs. Such systems could be utilized as catalysts for asymmetric hydrosilylation, anion-responsive ligand platforms for transition-metal coordination, as well as planar chiral Lewis pairs for small molecule activation.



Scheme 1. Modification of Lewis acid structure through metal and ligand substitution.

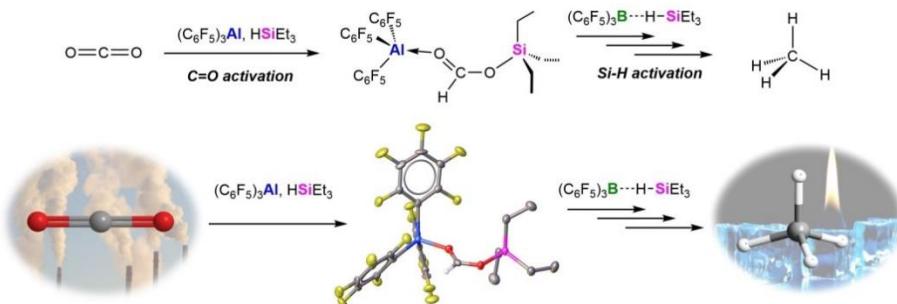


Figure 1. Catalytic hydrosilylation of CO_2 to CH_4 with the tandem $\text{B}(\text{C}_6\text{F}_5)_3/\text{Al}(\text{C}_6\text{F}_5)_3$ system.

AEI 42

The secondary building unit as metalloligand: Structural and mechanistic insight into catalysis at metal-organic framework nodes

Robert Comito, rcomito@mit.edu. Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States

Conventional heterogeneous catalysts are structurally inhomogeneous, providing a multiplicity of transition metal sites that complicate structural and mechanistic analysis. By contrast, the nodes of metal-organic frameworks (MOFs) offer a monodisperse and well-defined coordination environments for transition metals. In this lecture, I show that MOF catalysts prepared by cation exchange are tractable through a range of spectroscopic techniques and can be modeled effectively with molecular complexes. Using these tools, we demonstrate that the local coordination geometry of the MOF node is preserved through cation exchange, representing a predictable metalloligand-like platform for heterogeneous catalysis. Analyzing the polymerization and oligomerization of light alkenes with these MOFs, we characterize the basis for stereo- and regioselectivity, as well as the mechanisms of activation and deactivation.

Low temperature growth of $\text{ZrSe}_2/\text{HfSe}_2$ thin film and nanostructured complex metal chalcogenide MnSb_2Se_4

Honore Djieutedjeu¹, *hdjieutedjeu@yahoo.fr*, **Beth S. Guiton**¹, **Melonie Thomas**², **Yu Lei**³. (1) Chemistry, University of Kentucky, New Albany, Indiana, United States (2) Chemistry, University of Kentucky, Lexington, Kentucky, United States (3) Chemistry, University of Kentucky, Lexington, Kentucky, United States

The energy crisis and critical need of advanced materials for engineering, pharmaceutical and medical applications are calling for development of new materials to response quickly and efficiently to such demand. For such imperative request, the fundamental understanding of materials, the origin of the properties in correlation with structure could be the main pathway toward the successful design and discovery. Furthermore, the 2D metal dichalcogenides materials and their Heterostructures are promisingly reducing the gap between materials fit to the requirement for energy storage and harvesting. Recently, a new low symmetry of complex metal chalcogenide as MnSb_2Se_4 , FeSb_2Se_4 and MnBi_2Se_4 [1] with fascinating magnetic and transport properties has been reported with narrow band gap tunable upon doping. But, the nanostructure and thin film of such materials is not yet explored and which could set them as candidate for photodetection like $\text{Cu}_2\text{ZnSnS}_4$ and $\text{Cu}_2\text{ZnSnSe}_4$ [2]. The thin layer growth of 2D graphene like materials and particularly the transition metal chalcogenides (TMDCs) has been so far successful with metal oxide precursor at very high temperature [3]. Which may not absolutely offer the flexibility in controlling the size of the flakes and the thickness. We are reporting new ultra-fast low temperature synthesis of HfSe_2 , ZrSe_2 and $\text{ZrSe}_2/\text{HfSe}_2$ heterostructure. We demonstrate the possibility of tuning and controlling the thickness of the film and heterostructure by exploring range of temperature and gas flow rate. Thin film are characterized using the Raman spectroscopy, High resolution TEM and Atomic Force Microscope. Our result demonstrate that we successfully growth HfSe_2 or ZrSe_2 in the fewest layers flake reported and these two compounds are reported with interesting FET properties with device made with 14 layers [4]. We used two step chemical vapor deposition(CVD) to generate $\text{ZrSe}_2/\text{HfSe}_2$ heterostructure with potentials application in field effect transistor. We are reporting also, the CVD growth and characterization of MnSb_2Se_4 nanostructured catalyzed by the Au nanoparticle on Si substrate. The nanostructure of MnSb_2Se_4 exhibit various nanowire and nanorod morphologies.

Journey of macrocyclic proportions: From developing transition metal contrast agents to expanding the capabilities of porphyrinoid systems containing non-pyrrolic heterocycles

Sarina J. Dorazio¹, *sdorazio@buffalo.edu*, Christian Bruckner³, Franc Meyer². (1) Institut für Anorganische Chemie, Georg-August-Universität Göttingen, Göttingen, Germany (2) Univ Gottingen Anorgan Chem, Gottingen, Germany (3) Univ of Connecticut, Storrs Mansfield, Connecticut, United States

Research efforts and training in both organic and inorganic laboratories have shaped my independent research objectives through the synthesis of macrocycles as either the molecules of interest or as ligands for metal complexation. Highlights of this training include development of transition metal based macrocyclic contrast agents for MRI, multi-step synthesis and characterization of pyrrole-modified porphyrins (porphyrinoids containing at least one non-pyrrolic building block), and multi-step synthesis and characterization of expanded porphyrin metal complexes. My independent research efforts will emphasize synthetic organic and inorganic techniques. Merging expertise and interests in synthetic organic porphyrinoid chemistry with coordination chemistry, my independent research aims to develop synthetic strategies toward porphyrinoids and macrocyclic coordination complexes for applications as diverse as biomedical diagnostics and therapeutics, information storage, and light harvesting.

Unprecedented chromium-ligand multiple bonding and oxidative group transfer reactions supported by a macrocyclic N-heterocyclic tetracarbene

Gaya Elpitiya^{3,2}, *gelpitiy@utk.edu*, **David M. Jenkins**³, **Brian Malbrecht**¹. (1) 306M, Mallinckrodt, Cambridge, Massachusetts, United States (2) chemistry and Biochemistry, University of Southcarolina, Columbia, South Carolina, United States (3) Chemistry, University of Tennessee, Knoxville, Tennessee, United States

Metal-ligand multiple-bonds have long been of interest to organometallic chemists since they are the active intermediates for catalysis in oxidation reactions, such as epoxidation and aziridination. Particular attention has been paid to oxo, imido and nitrido complexes of earth-abundant first row transition metals, in particular iron, although little attention is given to earlier metals such as chromium. Most chromium complexes with these multiple bonds feature porphyrins or salens as auxiliary ligands, but these complexes have limited reactivity since they are high valent. A stronger s-donor ligand prepared by our group incorporating dianionic tetracarbenes combines the anionic charge of salen and porphyrin ligand systems with the improved s-donor strength of N-heterocyclic carbenes. This macrocyclic tetracarbene ligand platform stabilizes a rare electronically unsaturated, low valent, Cr(II) square planar complex that is highly reactive towards oxidants such as Me₃NO and organic azides. Different levels of steric bulk gives rise to chromium oxo, imido, and tetrazene complexes and the first example of a chromium m-nitrido species. The synthesis, structure and reactivity trends of these novel chromium tetracarbene complexes will be shown and this research is the most detailed study done on chromium-ligand multiple-bonding supported by a single auxiliary ligand platform.

AEI 46

Gold (I) sulfide nanostructures obtained via cation exchange of copper sulfides

Emil A. Hernandez-Pagan, *emil.a.hernandez@gmail.com*, **Janet Macdonald**. Department of Chemistry, Vanderbilt University, Nashville, Tennessee, United States

The family of I-VI semiconductor materials have garnered considerable attention as their opto-electronic properties and low toxicity make them attractive alternatives to Cd- and Pb-semiconductor based applications. Out of the I-VI family, the Cu and Ag sulfides have been extensively investigated and their synthesis and properties are well documented. In contrast, there have only been a few reports on the synthesis and characterization of gold (I) sulfide (Au₂S). The direct synthesis of Au₂S with suitable control over size and shape remains a challenge. Further, the metastable nature of the material once synthesized is a significant obstacle to the study of Au₂S, resulting in discrepancies on the properties reported. Here in, we report on the indirect synthesis of Au₂S via cation exchange from copper sulfide seeds. Both, Cu_{2-x}S (djurleite) and CuS (covellite), have been employed as starting point for the cation exchange. The cation exchange has been achieved in nanodisks and nanorods morphologies, resulting in Au₂S nanostructures that preserve the size and shape of the starting materials as determined by TEM. The conversion from copper sulfide to Au₂S was confirmed by XRD and Raman spectroscopy. Optical characterization was performed by UV-Vis absorption spectroscopy.

AEI 47

Nanoscale optimization of materials for optoelectronics

Matthew J. Jurow, *mjurow@Gmail.com*. University of Southern California, Los Angeles, California, United States

Molecular design and synthetic modification to control photonic properties and self-assembly of nanoscale architectures in electron donor, acceptor, transport materials and quantum confined nanocrystals will lead to a better understanding of how molecular structure affects interactions with light and charge in solid-state photonic materials.

My research spans organic, inorganic and organometallic materials and focuses on light-matter interactions. Materials we develop find applications in LED's and photovoltaics, but more critically generate basic understandings of the way light interacts with small molecules and nanocrystals.

AEI 48

Rhodium-cyanine fluorescent probes for detection and signaling of mismatches in DNA

Adela Nano², anano@caltech.edu, Jacqueline K. Barton¹. (1) Department of Chemistry, California Inst of Tech, Pasadena, California, United States (2) Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California, United States

Mismatched (non-Watson-Crick) base pair damage in DNA occurs naturally from errors during the replication process. Deficiencies in the mismatch repair (MMR) machinery, a DNA repair pathway, strongly predispose cells to cancer development. Therefore, efficiently detecting DNA mismatches will greatly enable early detection of MMR-deficient precancerous cells. Herein, we report the synthesis and characterization of a bifunctional fluorescent probe that combines a rhodium metalloinsertor with indol trimethine cyanine, Cy(3), the luminescent reporter, *via* a PEG-type linker. The conjugate displays low luminescence when free in solution or in the presence of well-matched DNA but exhibits a luminescence increase up to 9-fold in the presence of a 27-mer oligonucleotide containing a central CC mismatch. DNA photocleavage experiments demonstrate that upon photoactivation, the conjugate can cleave the DNA backbone near the mismatch site on a 27-mer oligonucleotide, thus providing further evidence for mismatch targeting. Fluorescence titrations of the Rh conjugate with genomic DNA (gDNA) extracted from MMR-deficient and MMR-proficient HCT116 cell lines show a luminescence differential between gDNA from MMR-deficient and -proficient cell lines, reflecting the sensitive detection of differences in mismatch frequency.

AEI 49

Nanomaterial synthesis using atomic layer deposition

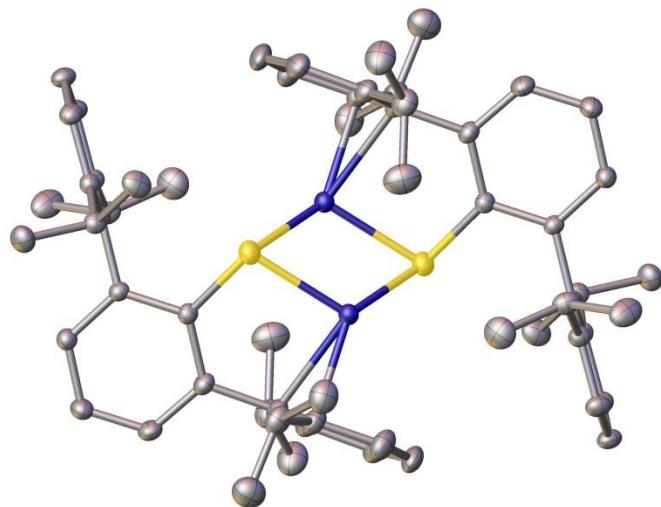
Sameer Patwardhan¹, sameerpatwardhan@gmail.com, George C. Schatz². (1) Argonne-Northwestern Solar Energy Research (ANSER) Center, Northwestern University, Evanston, Illinois, United States (2) Chemistry, Northwestern University, Evanston, Illinois, United States

Atomic layer deposition (ALD) is a thin-film deposition technique with applications in microelectronics and catalysis. More recently, its accessibility in academic labs is leading to rapid growth in the development of novel materials and methods with spatial precision of a single atom. I will present computational and experimental work involving the growth of inorganic clusters and nanoparticles (nps) on various substrates. In particular, I will discuss growth of MnO_x and ZnO nps on functionalized Au surfaces, and that of ZnO nps on the basal plane of graphene. Compared to thin-film growth, a controlled nanoparticle growth mode is turned-on by tuning surface properties of substrates. The nanostructures are characterized by spectroscopy and microscopy techniques, while computational modeling provides mechanistic details and ways to optimize growth.

Synthesis and characterization of homoleptic copper (I) thiolate complexes

Jade K. Pratt, *jadepratt@gmail.com*, **Philip P. Power**, Chemistry, University of California, Davis, Sacramento, California, United States

Research on copper–sulfur bonding remains of high interest primarily because of the presence of copper-sulfur bonded units in several copper containing proteins, their promising biological applications and as metal sulfide precursors for copper catalysts. Bulky terphenyl thiolato ligands were used in the stabilization of these copper complexes. In previous work, we and others have used terphenyl substituted thiolato ligands to stabilize various transition metal complexes with unusual coordination numbers. Recently, a homoleptic copper (I) thiolato complex, $(\text{CuSAr}^{\text{Me}6})_3$, was published by Walensky et. al. This copper thiolato trimer species features methyl substituents at the 2, 4 and 6 positions of the flanking terphenyl rings. Other published species include a heteroleptic anionic complex $\text{Cu}_3(\text{SAr}^{\text{iPr}6})_2\text{Br}$, which includes the very bulky $\text{Ar}^{\text{Pr}6}\text{S}^-$ ($\text{Ar}^{\text{Pr}6} = -\text{C}_6\text{H}_3-2,6-(\text{C}_6\text{H}_2-2,4,6-\text{Pr}^3)_2$) thiolato ligand with a bridging bromide ligand reported by Holm et al. Herein, we report the synthesis and characterization of a series of homoleptic copper thiolato complexes as exemplified by the tetrameric species $(\text{CuSAr}^{\text{t-Bu}2})_4$ ($\text{Ar}^{\text{t-Bu}2} = -\text{C}_6\text{H}_3-2,6-(\text{C}_6\text{H}_4-4-\text{tBu})_2$), $(\text{CuSAr}^{\text{Me}6})_4$ ($\text{Ar}^{\text{Me}6} = -\text{C}_6\text{H}_3-2,6-(\text{C}_6\text{H}_2-2,4,6-\text{Me}_3)_2$), as well as $(\text{CuSAr}^{\text{iPr}4})_2$ ($\text{Ar}^{\text{Pr}4} = -\text{C}_6\text{H}_3-2,6-(\text{C}_6\text{H}_3-2,6-\text{iPr}_2)_2$) which is the first structurally characterized dimeric copper thiolate complex. In addition, we describe the synthesis and characterization of the tricopper species $\text{Cu}_3(\text{SAr}^{\text{iPr}4})_2\text{I}$.



X-ray crystal structure for $(\text{CuSAr}^{\text{iPr}4})_2$. Copper (blue) atoms, sulfur (yellow) atoms and carbon (gray) atoms are shown. Hydrogen atoms are omitted for clarity, thermal ellipsoids are shown at 30% probability.

AEI 51

Those who wander are not lost, a two-continent academic journey: Molecular transformations by first-row transition metals, late transition metal organometallics, teaching, and establishing an independent research presence in contrast agents for MRI

Jeremiah J. Scepaniak¹, thesciencetype@gmail.com, Franc Meyer². (1) Institut für Anorganische Chemie, Georg-August-Universität, Göttingen, Niedersachsen, Germany (2) Univ Gottingen Anorgan Chem, Gottingen, Germany

An overview of research accomplishments throughout my academic training will be highlighted. Topics will include high-valent Fe complexes in relation to nitrogen atom transfer and nitrogen fixation, oxidation of 1° and 2° alcohols by M-TEMPO complexes (M = Fe, Al, B), forays into late transition metal organometallic chemistry and classroom teaching experience. This panorama will demonstrate experience in synthetic organic and inorganic chemistry, experimental design, and mentorship. These strengths in coordination chemistry will be used to merge experience in biomimetic chemistry with independent research interests regarding molecular transformations and design of contrast agents for MRI.

Sequential chemistry study of well-isolated and characterized quantum dots using batch and continuous flow platforms

Yi Shen, *yishen@mit.edu*. Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States

Colloidal semiconductor quantum dots (QDs) have attracted significant attention for applications spanning from display, photovoltaics to biological imaging because of their extraordinary photo-physical properties. In this presentation, I will first describe using gel permeation chromatography (GPC) as a media to purify different types of QDs. GPC is further demonstrated as a reactor to perform solvent change and ligand exchange reactions with QDs. With the help of GPC purification technique, well-isolated and characterized QDs are prepared to perform the sequential chemistry studies of these materials. (1) I specifically study the effect of neutral ligands on the photo-physical properties of the QDs and their influence on the inorganic surface overcoating (shell growth) reaction. (2) The GPC purified QDs are used to perform surface modification reactions with a range of polymeric imidazole ligands for biological imaging applications.

In the second part, I will describe recent advances using semiconductor nanoparticles prepared in continuous flow systems. (1) Matrix-assisted laser desorption/ionization (MALDI) characterizes the growth transition between clusters and nanoparticles in the late-stage growth of InP QDs. MALDI and NMR studies yield a size/extinction coefficient calibration curve for InP QDs without any assumption on the particles' density or shape. (2) Oscillatory flow reactor is used in automatically screening reaction conditions and studying the reaction mechanism of bi-phasic CdSe QD ligand exchange reactions. (3) Membrane-based in-line liquid-liquid extraction is efficient in removing impurities and excess precursors from nanomaterials as exemplified with continuous purification of CdSe QDs in octane.

AEI 53

Molecular to mesoscale: Identifying atomic-level structural features of nanocrystalline manganese oxides critical to understanding electrochemistry

Paul Smith¹, pfsmithjr@gmail.com, Amy C. Marschilok², Kenneth J. Takeuchi⁴, Esther S. Takeuchi³. (1) Rutgers University, Marlton, New Jersey, United States (2) SUNY Stony Brook University, Stony Brook, New York, United States (3) Stony Brook University, Stony Brook, New York, United States (4) Department of Chemistry, Stony Brook University, Stony Brook, New York, United States

This poster represents some of the presenter's Ph.D. and postdoctoral experiences regarding structure / function relationships among heterogeneous manganese oxides, homogeneous analogs, and their respective electrochemistries in two energy storage applications: 1) activity for catalytic oxidation of water and 2) capacity to reduce while intercalating Li^+ . For the former, the coordination geometry and oxidation state of the most likely catalytic manganese sites are proposed, as the result of a survey of ten manganese oxide polymorphs in two testing assays. For the latter, the relative roles of inter-particle vs. intra-particle electric conductivity of composite α - MnO_2 electrodes are probed through the chemical binding Ag^+ both within crystals and on the surface of crystals. One critical assertion is that discrete molecular manganese model compounds can provide insights for the electrochemistry observed on the material level.

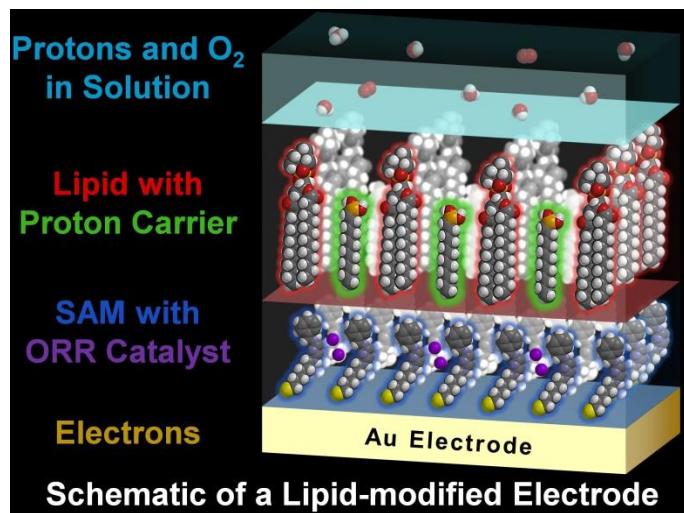
DNA damage recognition mediated by repair proteins carrying [4Fe4S] clusters and understanding proton-coupled electron transfer processes using a lipid-modified electrochemical platform

Edmund C M Tse¹, *etse@caltech.edu*, **Andrew Gewirth⁴**, **Thomas B. Rauchfuss³**, **Jacqueline K. Barton²**. (1) Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California, United States (2) Department of Chemistry, California Inst of Tech, Pasadena, California, United States (3) A131CSSL Box 60-6, University of Illinois, Urbana, Illinois, United States (4) Chemistry, University of Illinois at Urbana-Champaign, Urbana, Illinois, United States

In my postdoctoral work (Caltech), I unraveled the mechanism by which a collection of DNA-processing proteins containing redox-active [4Fe4S] metallocofactors detects DNA lesions and upholds genome integrity in a timely and synchronized fashion. DNA damage, as arise with defective repair, lead to cancer. I utilized electrochemistry, AFM, EPR, UV-Vis, CD, EMSA gel assay, and *in vivo* growth and rescue assay to understand the signaling and damage detection processes facilitated by [4Fe4S] enzymes with low cellular copy numbers. Experimental and biophysical modeling results validate a DNA damage search mechanism enabled by redox-active [4Fe4S] cluster proteins via long-range DNA-mediated charge transfer that explains the fast lesion detection kinetics observed in living organisms.

My PhD work (UIUC) includes facilitating and controlling the oxygen reduction reaction by using bio-inspired catalysts and so-called hybrid bilayer membranes (HBMs), which are self-assembled monolayers covered by a lipid layer. The latter work explores how HBMs supported on electrodes can be used to independently control the thermodynamics and kinetics of both proton and electron transfer processes in proton-coupled electron transfer reactions and thereby modulate the turover frequency and selectivity of catalysts.

Over the course of my academic training and research career, I have published 13 papers (with 6 additional manuscripts in preparation). My interests are broad, but center around self-assembly, electrocatalysis, synthesis, and protein and reaction dynamics. I have always enjoyed opportunities to conduct research that crosses traditional fields of study. My postdoctoral fellowship will end in July 2018 and I am eager and ready to start my independent academic career. Building upon a strong foundation in inorganic, analytical, and biological chemistry, I will devise new methodologies to understand reaction landscape in a complex environment and develop organic-inorganic hybrid platforms to promote efficient catalysis relevant to alternative energy conversion scheme.



AEI 55

High-valent organometallic nickel complexes mediated C-H bond activation and bond formation reactions

Wen Zhou, wenzhou@brandeis.edu. MIT, Cambridge, Massachusetts, United States

An atom-economic and step-economic aromatic cyanoalkylation reaction that employs nitriles as building blocks and proceeds through C_{sp^2} -H and C_{sp^3} -H bond activation steps mediated by Ni^{III} is presented. In addition to cyanomethylation with MeCN, regioselective α -cyanoalkylation was observed with various nitrile substrates to generate secondary and tertiary nitriles. Importantly, to the best of our knowledge these are the first examples of C-H bond activation reactions occurring at a Ni^{III} center, which may exhibit different reactivity and selectivity profiles than those corresponding to analogous Ni^{II} centers. Overall, these studies also provide guiding principles to design catalytic C-H activation and functionalization reactions involving high-valent Ni species.

From high valent Iron nitrides to catalytically relevant low valent homoleptic iron alkyl complexes

Salvador B. Munoz², smunoz4@ur.rochester.edu, **Michael L. Neidig**³, **Jeremy M. Smith**¹. (1) Indiana University, Bloomington, Indiana, United States (2) Chemistry, University of Rochester, Rochester, New York, United States (3) Department of Chemistry, University of Rochester, Rochester, New York, United States

The exceptional tunability of tris(carbene)borate ligands was demonstrated by the preparation of various nickel(II)nitrosyl complexes. Targeted modification of the ligand scaffold led to a host of steric environments as well as donation profiles that vary by more than 50 wavenumbers vNO. Additionally, high valent iron(IV)nitrides supported by strongly donating scorpionate ligands were found to react with a series of substituted styrenes, allowing for isolation of rare metal based aziridino complexes. The complete transfer of nitrogen atom to substrate was afforded by reaction of the aziridino with trimethylsilyl chloride affording a new synthetic path for synthetically valuable aziridines. While sterically bulky well-defined supporting ligands can allow for isolation of reactive moieties, limited access to the metal center can hinder turnover to effect a catalytic cycle. Catalytic systems lacking well-defined supporting ligands have been examined, namely those involving C-C bond formation by simple iron salts and alkyl Grignards developed by Kochi in the 1970's. These efforts have led to significant insights into identifying reactive intermediates in C-C coupling reactions such as homoleptic iron alkyl complexes. These highly unstable homoleptic organo-ferrates have been extensively studied spectroscopically and identified structurally by XRD. An eight iron cluster ($Fe_8Me_{12}^-$) which is highly reactive toward alkenyl halides is consistent with Kochi's observations ending a decades old mystery.

Cancer immunotherapy, cell imaging and drug delivery from self-assembled structure

Jae-Ho Lee, *leejaeho@mail.nih.gov*. NMD, RIS, Clinical Center, NIH, Bethesda, Maryland, United States

Cancer immunotherapy, especially monoclonal antibody (mAb)-based solid tumor therapy, is challenging due to various parameters that can impede the tumor delivery and penetration of therapeutic agents. The antigen (Ag)-mediated tumor targeting of mAb may be hampered by the presence of shed antigen in blood circulation because a high shed antigen concentration in the blood could act as a decoy preventing mAbs from binding to antigens expressed on tumor cells. My research is directed toward development of immunotherapy and cancer treatment based on nanomedicine to overcome the challenges in cancer immunotherapy. My research results presented here include: 1. Cancer immunotherapy *via* radiolabeling and image analysis 2. Computer model development for cancer immunotherapy 3. Stem cell imaging. 4. Drug delivery from self-assembled structures. For cancer immunotherapy, the tumor and organ uptake of Cu-64 or Zr-89 amatuximab has been studied and computer models including pharmacokinetics were developed to simulate the biodistribution and tumor uptake of Cu-64 and immunotoxin therapy effects. These studies further can be extended to simulate animal experiments and clinical studies to evaluate therapy effects and tumor progress. Stem cell tracking is still vital to understand cell and disease fate. To understand better the biological activities, stem cell tracking by multimodal superparamagnetic iron oxide nanoparticle (SPION) is also presented. Drug delivery based on self-assembled structure especially with biopolymers, vesicles, and liposomes is presented. Future research will explore personalized therapy based on targeted delivery (e.g., using recombinant DNA, antibody and exosome-like liposome nanoparticles) and drug screening for cancer therapy, computer-aided therapy diagnosis and prediction, and cellular engineering. As a scientist, I joined as reviewers in many journals and performed reviewing activities. Currently I serve as editorial members in some journals. I had submitted K99 grant as a fellow to gain grant process and am preparing for grants.

Development of azole antifungal analogues to treat Hedgehog dependent cancers

Kelly A. Teske, kelly.teske@gmail.com, Jennifer R. Pace, Albert M. DeBerardinis, Matthew K. Hadden. Pharmaceutical Sciences, University of Connecticut, Storrs-Mansfield, Connecticut, United States

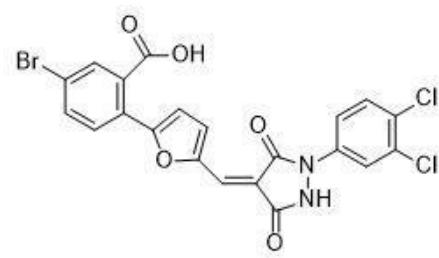
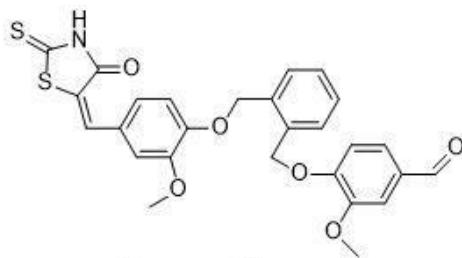
For the treatment of different cancers there remains a need for the design of targeted therapies that, unlike standard chemotherapies, block tumor growth at precise molecular targets without causing cytotoxic effects to healthy tissue. Although known for its role in regulating cell proliferation and differentiation during embryonic development, inappropriate activation of the Hedgehog (Hh) signaling pathway has been implicated in many cancers such as basal cell carcinoma and medulloblastoma. As a result, the Hh signaling pathway has emerged as a promising target for drug intervention. Itraconazole and Posaconazole are azole antifungals that have previously been identified as Hh-inhibitors with the ability to decrease tumor growth in models of Hh-dependent medulloblastoma. Using the azole antifungal scaffold, we report the specific structural modifications made to develop potentially potent Hh-dependent cancer therapies, herein.

Imparting intrinsic fluorescence as an approach towards rapid inhibitor screening and mechanistic evaluation of tuberculosis shikimate kinase

Rene Fuanta, rfn0001@tigermail.auburn.edu, **Douglas C. Goodwin**. Department of Chemistry and Biochemistry, Auburn University, Auburn, Alabama, United States

The shikimate pathway produces most compounds, most prominently, the aromatic amino acids. Shikimate kinase (SK) alongside other enzymes of the pathway are essential for viability of pathogens like *M. tuberculosis* (*M.tb*). The absence of a mammalian counterpart makes its enzymes attractive targets for development of new antitubercular agents. Our aim is to develop tools to rapidly identify SK inhibitors and characterize their mechanisms of inhibition.

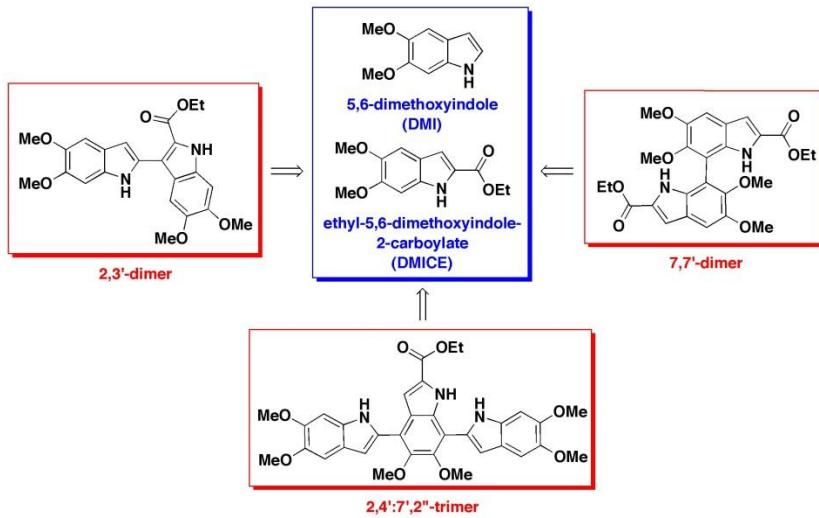
Interestingly, *M. tuberculosis* shikimate kinase (*MtSK*) is devoid of trp. Sequence alignments and structural studies were used to guide trp substitution on strategic sites in the enzyme. Three variants were: N151W (nucleotide-binding domain), E54W (shikimate-binding domain) and V116W (Lid domain). Kinetic parameters (ATP- and shikimate-dependent) of all three variants were similar to wild-type. The three variants showed characteristic and distinct trp emission spectra. ATP titration produced hyperbolic decreases in fluorescence emission were observed for all variants, with K_{DS} ranging from 0.2 - 0.4 μ M, similar to the apparent K_M for ATP. In contrast, titration with shikimate produced no change in fluorescence emission by either E54W or N151W *MtSK*, but there was a 30% decrease in V116W emission intensity in the presence of shikimate. V116 is part of the conformationally dynamic lid domain. This observation may point toward shikimate-induced conformational changes in *MtSK*. We also evaluated two inhibitors (see below). This is also corroborated by fluorescence anisotropy data. Both compounds produced a hyperbolic decrease in fluorescence intensity. K_{DS} for Compound 1 ranged from 16 to 33 μ M depending on the variant evaluated. For each variant, K_{DS} determined for compound 2 were about two fold lower than those of compound 1. ESI-LC-MS data suggest these inhibitors form no covalent adducts with the enzyme and dilution experiments also suggest a slow reversible mechanism is operating. Together, our data suggest that these variants will serve as valuable mechanistic probes of *MtSK* catalysis and inhibition



Towards a modular approach to Eumelanin oligomer synthesis

Andrew H. Aeby², aaeby@gmail.com, Jeff Levy¹, Benjamin Steger¹, Jason M. Belitsky¹. (1) Chemistry and Biochemistry, Oberlin College, Oberlin, Ohio, United States (2) Chemistry & Biochemistry, Oberlin College, Oberlin, Ohio, United States

Eumelanin, the black-to-brown pigment found in the human skin and hair, has recently inspired the development of a myriad of synthetic analogues with a variety of materials applications from organic semiconductors to modifiable surface coatings. The natural material and synthetic analogues are based on dihydroxyindole oligomers generated from oxidative polymerization. Despite the renewed interest in this biopolymer, the composition and supramolecular assembly of the oligomeric species remain poorly understood. At the predominantly undergraduate institution (PUI) Oberlin College, the Belitsky research group has been engaged in exploring the structure and non-covalent interactions involved in the formation of eumelanin. Working with two undergraduate students we have begun to develop modular synthetic schemes to systematically create a library of oligomers from commercially available 5,6-dimethoxyindole (DMI) and ethyl-5,6-dimethoxyindole-2-carboxylate (DMICE). The 5,6-dimethoxyindole starting materials were functionalized through a combination of regioselective halogenation, iridium-catalyzed borylation and Suzuki coupling chemistry. Specifically, DMICE has been monofunctionalized with aryl and heteroaryl substituents at the 3-position and difunctionalized at the 3,7- and 4,7-positions to create a series of novel 5,6-dimethoxyindole compounds, including biologically relevant indole dimers and trimers.



AEI 61

Exploring the scope of Lewis acid-catalyzed triplet energy transfer: [2+2] photocycloaddition and beyond

Mary E. Daub, *mdaub@uci.edu*, **Hawa Keita**, **Evan Sherbrook**, **Tehshik P. Yoon**. Chemistry Department, Univ of Wisconsin Madison, Madison, Wisconsin, United States

For over a century, Lewis acids have been known to alter the *singlet* excited states of organic compounds, and, until recently, their impact on the *triplet* excited states was largely unexplored. Since the initial disclosure from our laboratory that a chiral Lewis acid complex lowers the triplet energy of 2'-hydroxychalcones, we have determined that this mode of triplet-triplet activation is general for Lewis basic substrates. Using Stern–Volmer kinetics, we have shown that the formation of Lewis acid–Lewis base complexes activates fluorescence quenching of transition metal photosensitizers. While the ability to catalyze energy transfer to these complexes is general, harnessing the reactivity of the triplet excited states is substrate dependent.

AEI 62

Design, synthesis, and evaluation of *N*-phosphonacetyl-L-aspartate derivatives as putative human ATCase inhibitors

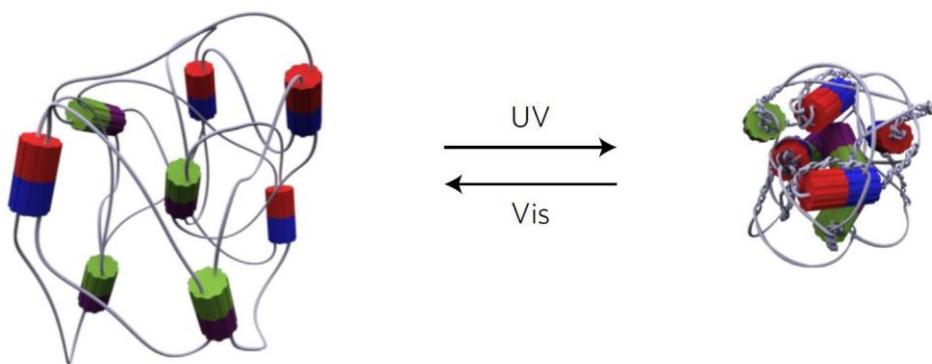
Mary Doud, *katiedoud@gmail.com*, **Caitlin Wolf**, **Kirsten Ponsart**. Chemistry, John Carroll University, University Heights, Ohio, United States

CAD is a multi-subunit enzyme formed by hexameric association of three functional domains: glutamine-dependent carbamoyl phosphate synthetase, aspartate transcarbamoylase (ATCase), and dihydroorotase. CAD catalyzes the first three steps in the *de novo* synthesis of pyrimidines, and its activity is essential to supply the high demand of nucleotides during cell growth and proliferation, making CAD a potential drug target for the development of cancer therapeutics. *N*-phosphonacetyl-L-aspartate (PALA) is a potent inhibitor of the ATCase domain. It is a transition-state analog of ATCase based on the structures of its two substrates, aspartate and carbamoyl phosphate, as well as the structure of the bacterial enzyme. The recent report of the first crystal structure of human ATCase, free and bound to PALA, provides insight into the inhibition of this subunit of CAD. In the human ATCase, only two of the three active sites show high affinity for PALA, offering new hints to understanding tumor resistance to PALA that plagued its clinical trials. Here we report the design, synthesis, and evaluation of a series of PALA derivatives as potential human ATCase inhibitors.

Dual-light control of nanomachines that integrate motor and modulator subunits

Justin T. Foy^{1,2}, justinfoy29@gmail.com, **Quan Li**², **Antoine Goujon**², **Jean-Remy Collard**², **Gad Fuks**^{2,3}, **Emilie Moulin**², **Olivier Schiffman**³, **Damien Dattlier**², **Daniel Funeriu**², **Nicolas Giuseppone**². (1) Chemistry, Bard College, Elizaville, New York, United States (2) CNRS - Institut Charles Sadron, Strasbourg Cedex 2, France (3) Mathematics, Univ. Paris Sud Saclay, Orsay, France

A current challenge in the field of artificial molecular machines is integrating multiple components into systems that can produce useful work when fueled with a constant source of external energy. A previous system from our lab composed of cross-linked, light-driven molecular motors contracted a gel material, however there was no reversible expansion of this gel. Here, we show that a multi-component gel composed of molecular motors and modulators, which respectively braid and unbraid polymer chains in crosslinked networks, it becomes possible to reverse their integrated motion at all scales. The photostationary state of the system can be tuned by modulation of frequencies using two irradiation wavelengths. Under this out-of-equilibrium condition, the global work output (measured as the contraction or expansion of the material) is controlled by the net flux of clockwise and anticlockwise rotations between the motors and the modulators.



Synthesis and characterization of functionalized heterocyclic compounds: 1,10-phenanthrolines and oxazoles

Sarut Jianrattanasawat, sarut.jianrattanasawat@wmich.edu, David L. Sellers, Elke Schoffers.
Department of Chemistry, Western Michigan University, Kalamazoo, Michigan, United States

Incorporation of heterocyclic moieties, such as an oxazole, can improve solubility, rigidity, and ability to accept hydrogen-bonds. Recently, our group showed the synthesis of oxazoles through a two-step procedure starting from an epoxide. First, an epoxide was opened in the presence of a Lewis acid to form a β -amino alcohol. This was followed by an oxidation using manganese dioxide. This method tolerates a variety of epoxide substrates, as well as a wide range of substituents at the 2-position of the oxazole. When other oxidizing agents were explored, such as *N*-bromosuccinimide (NBS) or 1,3-dibromo-5,5-dimethylhydantoin (DBDMH), we were able to chemoselectively oxidize the β -amino alcohol to oxazoline and 4-bromooxazoline, respectively. Structurally rigid compounds such as 1,10-phenanthroline offers insight into the oxidation mechanism. When NBS and DBDMH were used to oxidize 1,10-phenanthroline amino alcohol, only oxazoles were isolated.

Water-soluble cavitands: Applications in anion recognition and protein inhibition

Jacobs H. Jordan, jjordan2@tulane.edu, **Corinne L. Gibb**, **Bruce C. Gibb**. Chemistry, Tulane University, Destrehan, Louisiana, United States

The focus of this project has been two-fold: to synthesize novel container molecules capable of host-guest interactions exclusively in water – supramolecular systems driven by the hydrophobic and hofmeister effects – and to study their assembly profiles in aqueous solution. In this regard, we have utilized known deep-cavity cavitand octa-acid (OA) bearing eight negative charges as a model system for the design of analogous cavitands with orthogonal functionality: deep-cavity cavitands bearing pyridinium, ammonium and trimethylammonium groups were synthesized and characterized exhibiting similar binding motifs driven by the hydrophobic effect but containing two distinct binding sites capable of anion recognition. Moreover, novel systems, containing one analogous pocket were thus synthesized allowing for the attenuation of anion affinity and host solubility. These hosts contain varying degrees of hydrophobicity ultimately affecting their water-solubility and also their recognition properties, with potential implications towards sample purifications, and separations.

Additionally, application of OA as a potential protein-protein interaction (PPI) inhibitor with respect to the ATPase activity of simian virus 40 large T-antigen (sv40-TAg) was investigated. To probe enzymatic inhibition the focus is on a series of spectroscopic assays, which have shown potential inhibition of the ATPase activity of sv40-TAg at μM concentrations of OA. Based on MOE docking simulations, we posit that OA orients towards several His, and Arg residues in the central TAg channel resulting in protein inhibition. We will further discuss the potential for assay interference and the possibility for OA serving as a host to bind other assay components. OA is known to form dimeric capsules and 1:1 host-guest complexes in aqueous solution while in this work OA serves as a small molecule inhibitor of protein-substrate interactions in a larger supramolecular system. In addition, the enzymatic inhibition by OA was examined as the free monomer, the free monomer with strongly bound guest, and as the dimeric capsule. Inhibition was monitored in reference to low-dose controls and assays were screened for positive and negative interference with positively charged controls.

Ultimately, these results suggests modes of addressing the specific needs of supramolecular chemists by addressing the water-solubilizing groups of the host molecule to bring about specific solubility, affinity, and selectivity.

AEI 66

Synthesis of skeleton of bromophycolide A and D asymmetric homocrotylation of aldehydes rapid total synthesis of ciprofloxacin hydrochloride in continuous flow

Hongkun Lin, hongkunlin@gmail.com. MIT, Cambridge, Massachusetts, United States

In the first part, I will describe a concise asymmetric approach to the skeleton of bromophycolide A and D, in seven linear steps, 4 % overall yield, from known geranylgeranyl benzoate. This approach demonstrates (1) sequential functionalization of three out of the four alkenes from starting geranylgeranyl benzoate, (2) a highly regio and diastereoselective transannular cyclization, which differentiates three nearly identical alkenes in a macrolactone, controlled by a remote stereocenter and the conformation of this macrolactone.

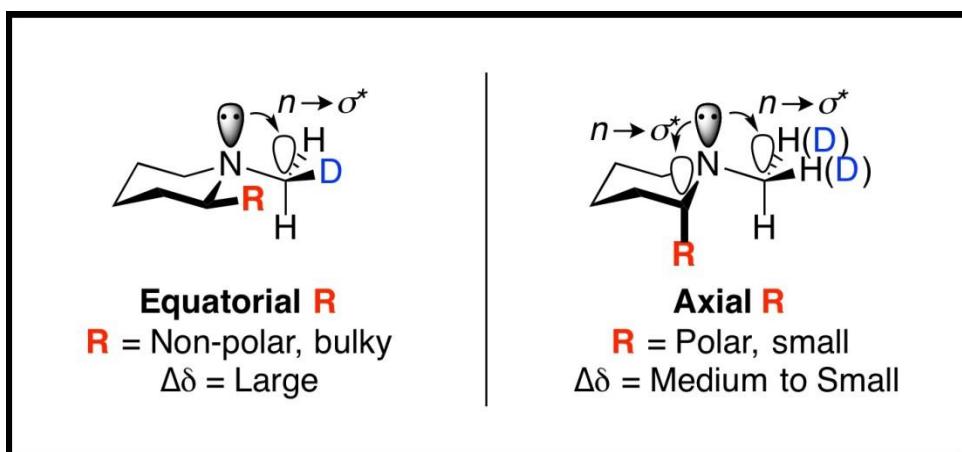
In the second part, I will describe a set of highly enantioselective and diastereoselective homocrotylation reagents and their enantiomers via cyclopropanation of vinylboronates, using tartaramide as an auxiliary and an additive. This set of reagents demonstrates broad substrate scope and functional group compatibility. The utility will be demonstrated in a concise modular formal synthesis of natural product (–)-spongidepsin.

In the last part, I will describe synthesis of rufinamide and ciprofloxacin in continuous flow. In recent years, continuous flow synthesis has emerged as a unique and efficient technique in synthetic chemistry. Rufinamide is an antiepileptic agent used to treat Lennox-Gastaut syndrome with brand names Banzel or Inovelon. Ciprofloxacin is on the World Health Organization List of Essential Medicines. It belongs to the family of fluoro-quinolone antibiotics and is used to treat a number of types of bacterial infections.

Toward the origin of small chemical shift differences in diastereotopic X-CH₂D groups

Onyekwere Ogba¹, maduka.ogba@gmail.com, **Stuart Elliott**², **David Kolin**¹, **Lynda J. Brown**², **Sebastian Cevallos**¹, **Malcolm Levitt**², **Daniel J. O'Leary**¹. (1) Department of Chemistry, Pomona College, San Gabriel, California, United States (2) Chemistry, University of Southampton, Southampton, United Kingdom

The proton pair of the CH₂D group in a chiral molecule are diastereotopic, yet only rarely exhibit different nuclear magnetic resonance (NMR) chemical shifts. Molecules that have a shift difference couple a locally asymmetric magnetic environment, with a CH₂D rotamer equilibrium perturbed by a secondary isotope effect caused by a selective weakening of methyl C-H(D) bonds by $n \rightarrow \sigma^*$ hyperconjugation. We have recently shown that a small proton chemical shift difference in *N*-CH₂D methylpiperidine supports long-lived nuclear spin states (LLS). Molecules like this may provide the opportunity to spin-tag methyl-containing molecules to study slow chemical processes, or use in functional magnetic resonance imaging applications. To identify additional candidate molecules with CH₂D groups exhibiting LLS and to investigate the factors governing its magnitude, we present a computational and experimental investigation of methyl rotational dynamics and proton chemical shifts in *o*-substituted *N*-CH₂D-piperidines. We show that stereoelectronic effects of the *o*-substituents on the piperidine ring strongly influence the ability to produce appreciable proton chemical shift differences in the *o*-substituted *N*-CH₂D piperidine family. The polarity and size of the *o*-substituent affects the 1,2-stereosiomeric relationship and consequently the strength of the rotational asymmetry within the *N*-CH₂D group.



AEI 68

Unprecedented reversible Buchner ring expansions by photochemically accessible triplet reactivity from a singlet DAC

Tharushi A. Perera, tabisheka.g@gmail.com. Chemistry, Texas state university, San Marcos, Texas, United States

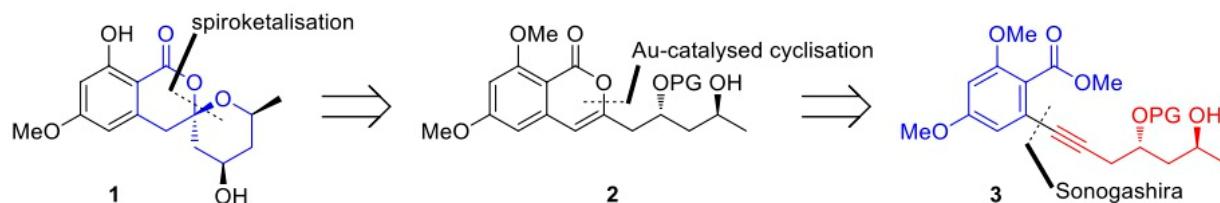
Carbenes are a fascinating class of divalent carbon atom-containing compounds with a high prominence in organic chemistry. Singlet carbenes are comprised of two paired valence shell electrons in one orbital which are not participating in any bonding interactions. Triplet carbenes, another electronic state of a stable carbene possesses two nonbonding electrons with parallel spins and are populated in different orbitals. Triplet carbenes are more challenging to obtain, however hold great promise to access distinct and complex structural motifs which are highly desirable in the field of organic chemistry, drug discovery and organic ferro-magnetics. We present the first example of an isolable free singlet carbene capable of achieving triplet reactivity via photochemically to form reversible Buchner ring expansion reactions. This new photochemical reaction allows a high-yielding reaction to versatile building blocks for chemical synthesis.

AEI 69

Total synthesis of citreoviranol

Rachelle Quach, rachellequach@gmail.com, **Daniel P. Furtkert**, **Margaret Brimble**. School of Chemical Sciences, The University of Auckland, Auckland, New Zealand

Citreoviranol (**1**) is a member of the biologically active resorcylic lactone family, isolated from the fungus *Penicillium citreoviride*. In addition to the characteristic resorcylic lactone moiety, citreoviranol also contains a very rare 6,6 spiroketal lactone. Prior to this work, a total synthesis and biological evaluation of this unique molecule had yet to be undertaken. Gold catalysis has proven to be a mild and efficient method for the synthesis of acid-sensitive spirocyclic heterocycles. Here, we present the total synthesis of citreoviranol using a gold catalysed cyclisation and a novel base induced spiroketalisation.



Scheme 1. Retrosynthetic analysis of citreoviranol (**1**)

AEI 70

Introducing undergraduate researchers to organic electronics

Julia A. Schneider, *julia.schneider@mail.mcgill.ca*. MRL, University of California, Santa Barbara, Santa Barbara, California, United States

Organic electronics are a class of devices in which molecules or polymers serve as the electrically active material. Notably, the properties of these organic materials can be endlessly tuned through structural modifications and tailored for a specific application. Solution-processable materials offer the possibility of inexpensive, printed devices, including solar cells, light-emitting diodes, and transistors. Such devices made entirely from biodegradable materials could additionally help stem the accumulation of e-waste in landfills. In all these applications, the morphology of the material is crucial to device performance. While some design strategies yield predictable results, many structure-property relationships are not well understood, especially as they relate to supramolecular ordering.

The presented work will feature research on a variety of projects well suited to introduce organic electronics to undergraduate researchers. Conjugated polymers bearing $-\text{SR}$ and $-\text{SO}_2\text{R}$ side chains will be presented, wherein the energy levels and the fluorescence of the material can be tuned by changing the oxidation state of the side chains.

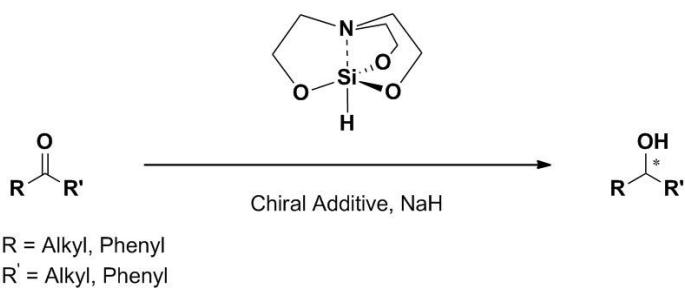
The effect of these side chains on the morphology of materials will also be studied in small molecules. By functionalizing organic semiconductors with cyclohexylsulfanyl and cyclohexylsulfonyl groups, for example, the electronic properties of the molecules could be tuned while exploring possible liquid crystalline behavior and changes in film morphologies.

Students will also have the opportunity to synthesize entirely novel semiconductors. Through the visible-light activation of vinyl azides, we will attempt to synthesize azepine containing organic semiconductors. As with all our materials, these semiconductors will be fully characterized using a variety of techniques, including UV-vis absorption, fluorescence, gel permeation chromatography, and electrochemistry.

1-Hydrosilatrane: A chiral Lewis base activated reducing agent for the asymmetric reduction of prochiral ketones to alcohols

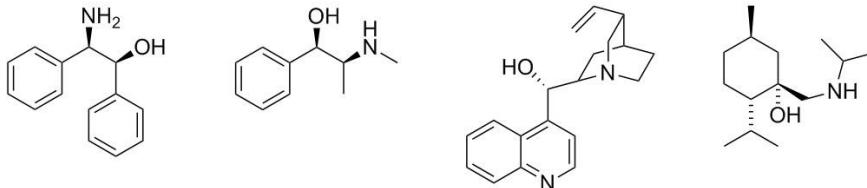
Sami Varjosaari, *sami.varjosaari@hotmail.com*, **Vladislav Skrypai**, **Thomas M. Gilbert**, **Marc J. Adler**. Chemistry & Biochemistry, Northern Illinois University, DeKalb, Illinois, United States

The reduction of prochiral ketones to chiral alcohols is a quintessential functional group manipulation in organic chemistry. 1-Hydrosilatrane – a robust, inexpensive, easy to handle alkoxysilane derivative – has been shown to reduce carbonyls in the presence of Lewis base activators. Therefore an appropriate chiral Lewis base could potentially induce enantioselectivity in prochiral ketones. With this in mind, we have been able to obtain fair to excellent enantioselectivity using deprotonated chiral amino alcohols as activators. For example, acetophenone was reduced to (R)-phenylethanol with up to 99% yield and 85% *e.e.*



R = Alkyl, Phenyl
 R' = Alkyl, Phenyl

Examples of Chiral Additives:



Vibrational modes involved in the function of the major light-harvesting complex of higher plants investigated by femtosecond-stimulated Raman spectroscopy

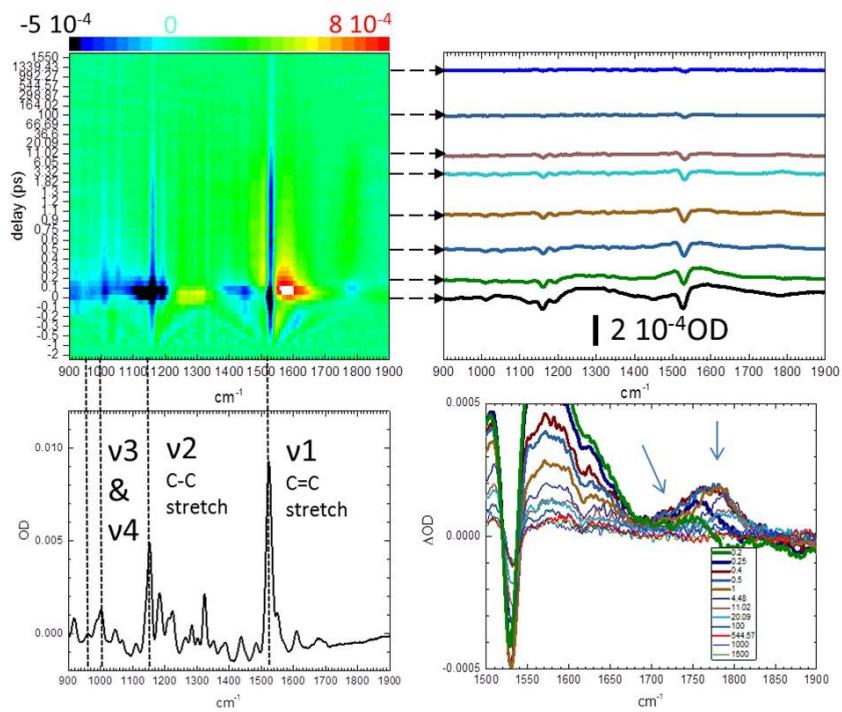
Juan Manuel Artes Vivancos, *j.m.artesvivancos@vu.nl*. Chemistry, University of California Berkeley, Amsterdam, Netherlands

Understanding the mechanisms that modulate photosynthesis is a challenge in biophysics and chemistry, and obtaining that knowledge could help for the design of highly-efficient light-conversion devices. We have used fs-Raman spectroscopy to study trimeric Light-Harvesting Complexes from higher plants, obtaining the dynamics of the vibrations of the pigments with femtoseconds temporal resolution. Herein, we show the first time-resolved results of the vibrational modes of xanthophylls and chlorophylls in the excited state of Light-Harvesting Complexes. By selectively exciting groups of pigments, we obtain the time evolution of their vibrational spectra (fig 1) and relate them to the light harvesting mechanism.

When exciting carotenoids, we observe ground state bleach (GSB) of the main vibrational modes of these molecules, as well as positive bands in good agreement with vibrational modes reported for the S1/S* states of pure carotenoids in organic solutions in the literature. The spectra show an extremely long-lived species that has spectral characteristics corresponding to a triplet state. This evidence suggests a possible singlet fission process in the LHCII from plants.

Experiments at different actinic pumps allow to selectively excite different carotenoids in the complex and global analysis of the data shows extended lifetime for distorted or cis carotenoids. When exciting chlorophyll at 675 nm, GSB in vibrational modes corresponding to the breathing of the ring are obtained. Remarkably, there is simultaneous GSB for the same carotenoid modes obtained in previous experiments. This indicates that the different pigments are coupled and that excitation is quickly delocalized over several different pigments in the complex.

These results constitute a proof of concept of the application of fs-Raman to complex photosynthetic samples and pave the way for future research aiming for a complete model of the light harvesting mechanisms in photosynthesis and their regulation.



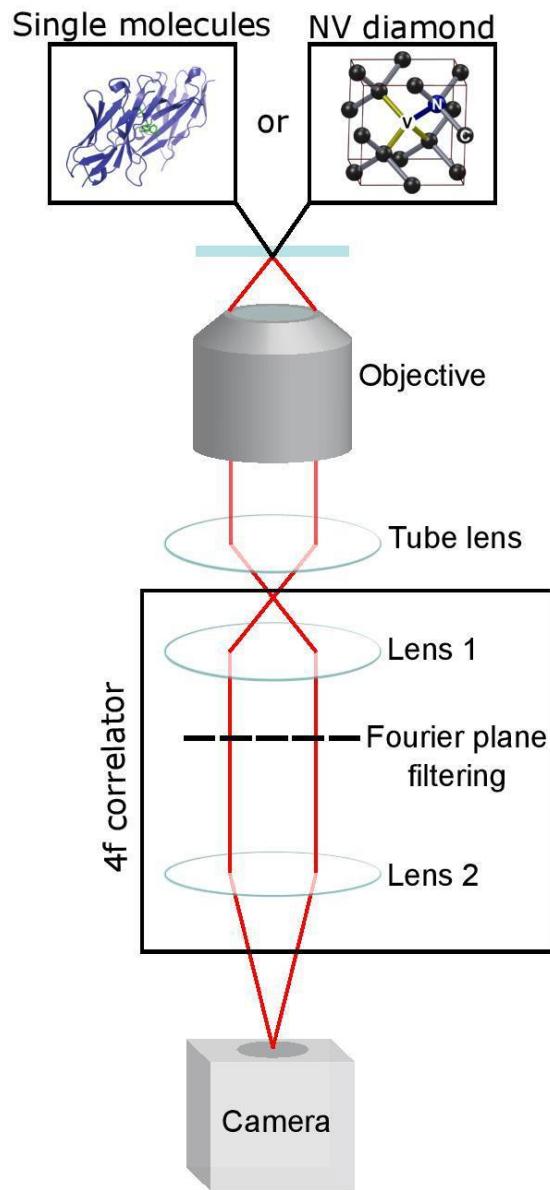
Single molecules, metamaterials, and diamond magnetometry: Novel approaches in Fourier optical microscopy

Mikael P. Backlund^{1,3}, *mpbacklund@gmail.com*, **Amir Arbabi**², **Petar N. Petrov**⁴, **Pauli Kehayias**^{1,3}, **Ehsan Arbabi**², **Saumya Saurabh**⁴, **Andrei Faraon**², **Ronald L. Walsworth**^{1,3}, **William E. Moerner**⁴. (1) Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts, United States (2) T. J. Watson Laboratory of Applied Physics, California Institute of Technology, Pasadena, California, United States (3) Department of Physics, Harvard University, Cambridge, Massachusetts, United States (4) Department of Chemistry, Stanford University, Stanford, California, United States

Fourier optical engineering constitutes a powerful suite of imaging techniques. By modulating collected light at the Fourier plane of the microscope (Fig. 1) one can simultaneously access all points in the image in order to correct errors or improve parameter estimation. We present two studies that make use of such methods, fostering new capabilities in microscopy.

The first study concerns nanoscale localization of single fluorescent molecules, a crucial function in advanced microscopy techniques including single-molecule tracking and super-resolution imaging. Molecules emit anisotropically, which can cause significant localization biases using common estimators. We demonstrate a solution to this problem based on azimuthal polarization filtering at the Fourier plane using a high-efficiency dielectric metasurface device composed of elliptical nanoposts. We recover nanoscale localization accuracy both for fluorescent dyes embedded in a polymer matrix, and for dL5 proteins binding malachite green.

The second study involves wide-field vector magnetic imaging with nitrogen-vacancy (NV) center ensembles in diamond. Typical magnetic imaging with NV ensembles requires a large applied magnetic field in order to resolve the spin resonances of different NV orientations. However, some samples cannot withstand such external fields. We leverage Fourier plane processing to separate the photoluminescence due to each NV orientation by optical means, enabling vector magnetic imaging without such a bias field. We apply our method to image magnetic fields of a thin slice from the Allende meteorite.



Computing nuclear quantum effects with the nuclear electronic orbital approach

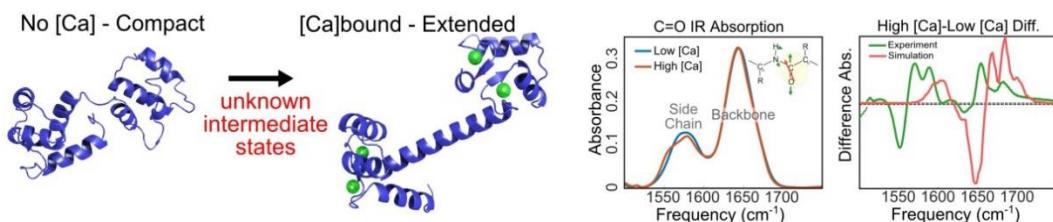
Kurt Brorsen, *kbrorsen@illinois.edu*. Chemistry, University of Illinois at Urbana-Champaign, Urbana, Illinois, United States

The nuclear electronic orbital (NEO) approach includes non-adiabatic and nuclear quantum effects for select nuclei by treating these nuclei quantum mechanically in a manner consistent to the electrons. Due to the attractive interaction of electrons and protons and the lack of electron-proton correlation, mean-field based NEO approaches give a much too localized nuclear density when compared to benchmark grid-based approaches. NEO approaches that include explicit electron-proton correlation give an accurate nuclear density along a single-dimension of a molecule, but require the computation of up to five particle integrals, severely limiting applicability. Additionally, explicitly correlated NEO approaches have difficulty computing accurate nuclear densities in all dimensions for adiabatic systems due to limitations of the explicitly correlated NEO ansatz. Because of these difficulties, recent NEO research has focused on the development of multicomponent (MC) density functional theory (DFT) functionals. One recently developed functional, based on the Colle-Salvetti formulation of the correlation energy, has shown the ability to reproduce the density of grid-based approaches, while having similar computational scaling to that of standard electronic DFT. This MC-DFT approach allows for the inclusion of nuclear quantum effects for a wide variety of chemical applications. A brief overview of wavefunction and DFT based NEO approaches, the ability of these approaches to compute nuclear densities, and initial chemical applications of the Colle-Salvetti based NEO-DFT functional will be presented.

Revealing the dynamics that control protein and biomolecule activity using FTIR and ultrafast 2DIR spectroscopy in combination with molecular dynamics simulations

Sean C. Edington, seanedington@gmail.com. Chemistry, University of Texas at Austin, Austin, Texas, United States

The rapid structural changes, termed “conformational dynamics,” that proteins experience as they perform their biological functions play a critical role in both the normal operation and pathogenic dysfunction of many biological processes and pathways. Despite their importance, these dynamics remain poorly understood even after close study because they are exceedingly difficult to probe experimentally. Fourier transform infrared (FTIR) spectroscopy, ultrafast two-dimensional infrared (2DIR) spectroscopy, and molecular dynamics (MD) simulations were used to investigate the conformational dynamics of calmodulin (CaM). CaM is a Ca^{2+} -signaling molecule expressed in every eukaryotic cell, responsible for controlling hundreds of other proteins and cellular functions, and whose mutations cause life-threatening cardiac disease. This investigation probed CaM's structural response to the presence of Ca^{2+} and a series of trivalent lanthanide ions on the native timescales of protein rearrangement. 2DIR spectroscopy, combined with MD simulations, provides both the time resolution and structural specificity necessary to build a picture of fast structural change in proteins, which has not previously been possible. Studying CaM's response to unnatural ligands such as the trivalent lanthanides in addition to the native ligand, Ca^{2+} , provides a window into how subtle perturbation of binding site geometry cascades through CaM's structure to induce other conformational changes. This research program provides new insights into how fast conformational dynamics drive CaM activity and specificity and suggest how even minor changes to protein primary structure critically disrupt the protein's dynamic behavior and lead to disease.



Both the bound and unbound structures of calmodulin are well characterized, but the intermediate states separating these conformational endpoints are unknown, as are the conformational excursions made by the protein as it undergoes thermal fluctuations. FTIR and 2DIR spectroscopy are well-suited to probing these critical structural changes.

Wide-field super-resolution infrared microscopy for aquatic pollutant examination

Brynnna Jones, jone1674@umn.edu. Materials Measurement Laboratory, National Institute of Standards and Technologies, Gaithersburg, Maryland, United States

Synthetic fibers are emerging as an important problem in aquatic pollution. To examine the presence, activity, and fate of these pollutants, a technique is needed that has spatial and temporal chemical specificity. The wealth of information contained in the mid-IR region of the electromagnetic spectrum is staggering. This is the location of the “fingerprint” region, well-known to contain characteristic vibrational signatures for a wide variety of compounds. In addition, IR spectroscopy also yields quantitative information. IR microscopy, therefore, reveals what substances are in the sample, how much is present, and where they are located. Performing this microscopy in a wide-field configuration, where the entire image is acquired at one time, adds temporal specificity. Using structured illumination, the resolution of the instrument (always a concern in the infrared) can be increased by up to a factor of two. There are three different operational modalities in which such an instrument will be developed and brought to bear on the problem of plastic fiber contamination. Hyperspectral imaging, the first mode, gives a spectrum at each pixel of the image. It thus combines chemical and spatial information. The second mode is time-course imaging, where the wavelength is fixed at a specific value and monitored over time. This mode would be used for kinetics studies examining leaching from or reactions with the fibers. Super-resolution imaging would be the third mode, giving increased spatial information.

Photochemical dynamics for intramolecular singlet fission in covalently-bound pentacene dimers

Zhou Lin, *linzhoubunny@gmail.com*, **Hikari Iwasaki**, **Troy A. Van Voorhis**. Department of Chemistry, Massachusetts Institute of Technology, Allston, Massachusetts, United States

In organic photovoltaics (OPVs), singlet fission (SF) converts a singlet exciton (S_1) into a pair of triplets (T_1), $S_1 \rightarrow ^1(T_1T_1) \rightarrow 2T_1$, and doubles the electric current generated by incident high-energy photons. A pentacene-based OPV allows the exothermic and spontaneous SF reaction to happen and its solar conversion efficiency can exceed the Shockley–Queisser limit of 33.7%. SF undergoes via a mysterious, “multi-exciton (ME)” intermediate, for which the character is still under debate for the lack of strong supports from ultrafast quantum dynamics. Based on many popular hypotheses, ME has a large charge transfer (CT) character but is also strongly coupled to S_1 and $^1(T_1T_1)$. As a unimolecular reaction, intramolecular SF (ISF) occurring to covalently-bound pentacene dimers provides an excellent model for local excitons and simplifies the studies of direct quantum dynamics.

In the present study, the ISF mechanism is investigated for three dimeric species, *ortho*-, *meta*-, and *para*-bis(6,13-bis(triisopropylsilyl)pentacene)benzene, in three different environments: vacuum, implicit solvent, and explicit solvent. The real-time, non-adiabatic quantum mechanical/molecular mechanical (QM/MM) dynamics is propagated among multiple potential energy surfaces associated with the diabatic, SF-relevant states -- S_1 , $^1(T_1T_1)$ and CT. The energy difference and non-adiabatic coupling between each pair of states fluctuate significantly with time and instantaneous molecular configurations. Condon and non-Condon ISF dynamics obtained from the present study are also quantitatively compared with solution-based experimental data. The results are expected to decipher the roles of ME and CT states in the ISF mechanism and propose a design strategy to maximize the ISF efficiency in the OPV materials.

Crystal orientation dependence of heterogeneous nucleation at the Cu-Pb solid-liquid interface

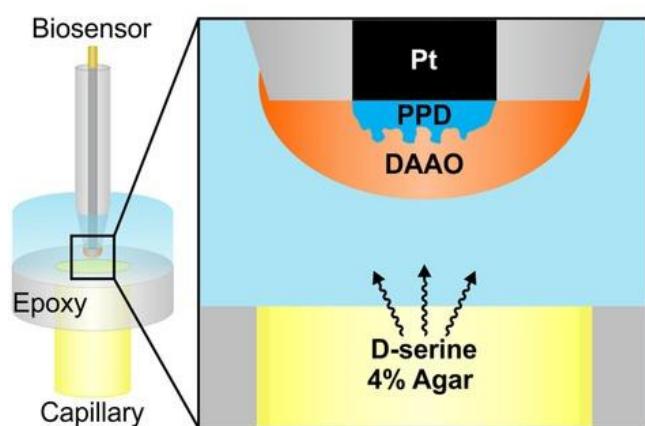
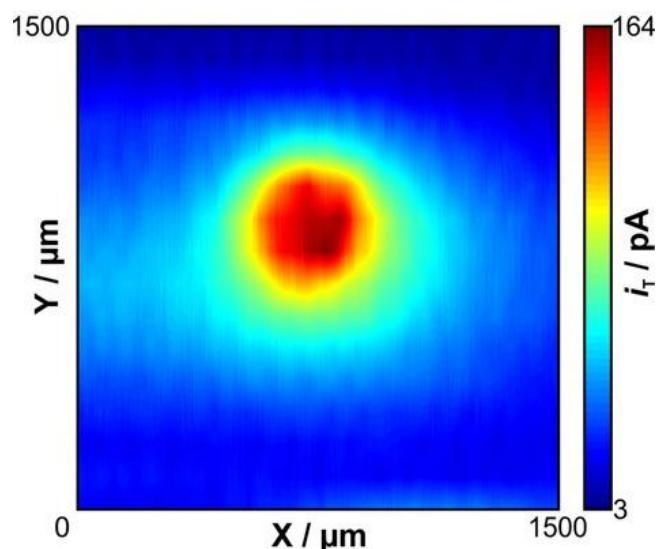
Pablo Palafox¹, *pablo.palafox49@gmail.com*, **Brian Laird**². (1) Chemistry, The University of Kansas, Lawrence, Kansas, United States (2) University of Kansas, Lawrence, Kansas, United States

In this work, we examine the effect of surface structure on the heterogeneous nucleation of Pb crystals from the melt at a Cu substrate using molecular-dynamics (MD) simulation. In a previous work [Palafox-Hernandez et al., *Acta Mater.* 59, 3137 (2011)] studying the Cu/Pb solid-liquid interface with MD simulation, we observed that the structure of the Cu(111) and Cu(100) interfaces was significantly different at 625 K, just above the Pb melting temperature (618 K for the model). The Cu(100) interface exhibited significant surface alloying in the crystal plane in contact with the melt. In contrast, no surface alloying was seen at the Cu(111) interface; however, a prefreezing layer of crystalline Pb, 2-3 atomic planes thick and slightly compressed relative to bulk Pb crystal, was observed to form at the interface. We observe that at the Cu(111) interface the prefreezing layer is no longer present at 750 K, but surface alloying in the Cu(100) interface persists. In a series of undercooling MD simulations, heterogeneous nucleation of fcc Pb is observed at the Cu(111) interface within the simulation time (5 ns) at 592 K—a 26 K undercooling. Nucleation and growth at Cu(111) proceeded layerwise with a nearly planar critical nucleus. Quantitative analysis yielded heterogeneous nucleation barriers that are more than two orders of magnitude smaller than the predicted homogeneous nucleation barriers from classical nucleation theory. Nucleation was considerably more difficult on the Cu(100) surface-alloyed substrate. An undercooling of approximately 170 K was necessary to observe nucleation at this interface within the simulation time. From qualitative observation, the critical nucleus showed a contact angle with the Cu(100) surface of over 90 degrees, indicating poor wetting of the Cu(100) surface by the nucleating phase, which according to classical heterogeneous nucleation theory provides an explanation of the large undercooling necessary to nucleate on the Cu(100) surface, relative to Cu(111), whose surface is more similar to the nucleating phase due to the presence of the prefreezing layer.

Localized detection of D-serine by using an enzymatic amperometric biosensor and scanning electrochemical microscopy

David Polcari¹, Samuel Perry¹, samuel.perry@mcgill.ca, Loredano Pollegioni², Matthias Geissler³, Janine Mauzeroll¹. (1) Chemistry, McGill University, Montreal, Quebec, Canada (2) Dipartimento di Biotecnologie e Scienze della Vita, Universita degli studi dell’Insubria, Varese, Italy (3) Life Sciences Division, National Research Council of Canada, Boucherville, Quebec, Canada

D-Serine acts as an endogenous co-agonist for *N*-methyl-D-aspartate receptors at synapses, making it essential for proper brain development and function. This amino acid has also been linked to several neurodegenerative diseases such as Alzheimer's disease and dementia. Nevertheless, the primary site and mechanism of D-serine release remains unclear. We recently demonstrated the use of an enzymatic amperometric biosensor for the *in vivo* quantification of endogenous D-serine release in *Xenopus laevis* tadpoles. Herein, we investigate the effect of the permselective poly(*meta*-phenylenediamine) electropolymerization conditions on the biosensor's response time and selectivity. Scanning electrochemical microscopy (SECM) is then used with the optimized biosensor to measure localized release of D-serine from a model system. This SECM methodology, which provides high spatial and temporal resolution, could be useful to investigate the primary site and mechanism of D-serine release in other biological samples.

A**B**

SECM measurement of D-serine release. A) Schematic representation of the experimental configuration for SECM measurements using the biosensor. A capillary ($d = 300 \mu\text{m}$) is filled with 4 % agar containing 50 mM D-serine and embedded in an epoxy puck, which is inverted below the biosensor. B) SECM image of an embedded capillary containing D-serine ($E = 500 \text{ mV vs. Ag/AgCl}$; $a = 12.5 \mu\text{m}$; $v = 10 \mu\text{m s}^{-1}$).

AEI 80

Revealing the excitonic and structural properties of light-harvesting molecular assemblies through electronic-vibrational spectroscopy

Christopher C. Rich, *richcc@colostate.edu*. Chemistry, Colorado State University, Fort Collins, Colorado, United States

I am a postdoctoral researcher who is seeking a tenure-track faculty position at a research university where I can conduct a research program while actively mentoring graduate and undergraduate students. My research interests involve the investigation of the excitonic and structural properties of light-harvesting molecular assemblies using advanced spectroscopic techniques. Light-harvesting molecular aggregate have been a recent material of interest for implementation in less expensive photovoltaics and solar fuel devices. The formation of spatially delocalized excitons in these materials can result in photon absorbing and electron funneling properties similar to that of light-harvesting antennae of photosynthetic organisms. However, directly measuring the internal structure of some of the light-harvesting aggregates, particularly those with nanoscopic dimensions, can be challenging, even with advanced imaging techniques. Spectroscopic techniques have thus been used to convey information on both the structural and excitonic properties of these systems. Extending upon the work I have accomplished as a postdoctoral researcher and as a graduate student, my future research plan will endeavor to derive new insights on light-harvesting aggregates using frequency- and time-resolved spectroscopies, including resonance Raman spectroscopy and microscopy, heterodyne-detected sum frequency generation spectroscopy, and impulsive stimulated Raman spectroscopy. Students and postdocs in my research group will engage in these spectroscopy techniques to uncover the underlying structure of these aggregates as they relate to their excitonic properties, including exciton-phonon coupling and exciton transport. Further I hope to use the results from these studies to encourage collaborations with other research groups to design new light-harvesting aggregates for materials to use in solar energy technology. Using an active, Socratic approach I have developed from my various teaching experiences, I hope to foster the next generation of scientists and science-literate citizens and encourage greater diversity in chemistry, physics, and other STEM fields.

AEI 81

Leveraging a computational chemistry app-store for both teaching and researching chemistry

Ryan Richard^{2,1}, ryanmrichard1@gmail.com. (1) Georgia Institute of Technology, Atlanta, Georgia, United States (2) Chemistry, Iowa State University, Ames, Iowa, United States

I am currently one of the lead developers of the Pulsar Computational Chemistry Framework which is a software project designed to impart an "app-store" like environment to computational chemistry. Pulsar has facilitated my past research and will be a key component in my future research interests. Aside from its research applications, it is my opinion that Pulsar can be a valuable teaching tool for physical chemistry and computational chemistry courses. This is because Pulsar provides a user-friendly interface to existing computational chemistry methods. Homework and lab assignments can have students tweak methods, like Hartree-Fock and density functional theory, in real time to explore how the changes affect energies, orbitals, molecular geometries, etc. This same interface can also be used to drive research quality computations allowing the student to gain theoretical insight for an accompanying experiment, in a familiar computing environment.

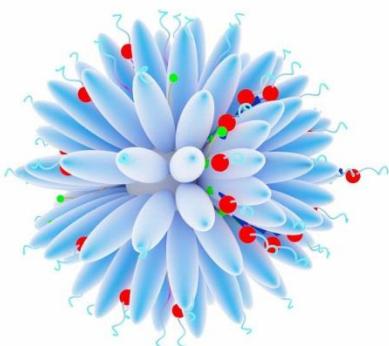
The majority of my past research has focused on fragment based methods, which are a series of computational chemistry methods that aim to extend the applicability and accuracy of existing quantum chemistry methods to comparatively large systems. My proposed research project will utilize fragment based methods to study molecular magnets, molecules which individually posses intrinsic magnetic moments. Consequentially, there is great interest in using these molecules in a variety of roles including quantum computing, electronic data storage (*i.e.* hard drives), and molecular machines. The ability to adsorb a molecular magnet on a surface, without it loosing its magnetic moment, is a prerequisite for most applications and at the moment a challenging experimental task. In my research proposal, I have devised a series of research projects, of varying difficulties, that over a five year period will allow my group to simulate and better understand the interactions occurring between the molecular magnet and the surface. With such knowledge I expect to aid experimental researchers in designing chemical systems in which the molecular magnet's magnetization persists.

Engineering the molecular interactions for biomedical applications

Handan Acar¹, hacar@uchicago.edu, Matthew V. Tirrell². (1) Institute for Molecular Engineering, The University of Chicago, Chicago, Illinois, United States (2) IME, University of Chicago, Chicago, Illinois, United States

Interest in peptides as potential drug candidates has naturally increased with recent progress in enhancing their structural and chemical stability, along with their ability to cross the cell membrane. Peptide-based therapeutics that target not only specific cells but also specific protein-protein interactions in the cytoplasm will herald a new era of “personalized medicine”. In this approaching new era, chemical tools to engineer peptides into molecular probes will be invaluable. The combination of carefully selected and localized interactions will produce stable assemblies, which can be reversible, highly tunable, dynamic, and modular as required by the specific application. Effective approaches to the design of molecular therapeutics must be safe, sensitive, efficient, and rapidly adapted to new targets with minimal effort and expense. To enable new translational clinical technologies, my research will focus on molecular design that incorporates these aspects into the new materials.

I sought to broaden the translational focus of my research during my postdoctoral work at Institute for Molecular Engineering at the University of Chicago with Matthew Tirrell, PhD. Taking advantage of the university’s rich mix of clinicians and translational scientists, I work closely with James LaBelle MD, PhD, a pediatric oncologist in the Pritzker School of Medicine whose research involves peptide therapeutic translation to refractory malignancies. This cutting-edge collaboration between myself, Dr. Tirrell and Dr. LaBelle led to the development of a self-assembled nanoparticle platform, comprised of enzymatically cleavable peptide amphiphiles, that carries therapeutic peptides into cells. This platform offers the unique ability to follow intracellular drug trafficking and enzymatic cleavage in real time. The broad-ranging application of this technology to clinical medicine, biochemical research, and peptide-based nanoparticle development led us to file a patent application through the University of Chicago.

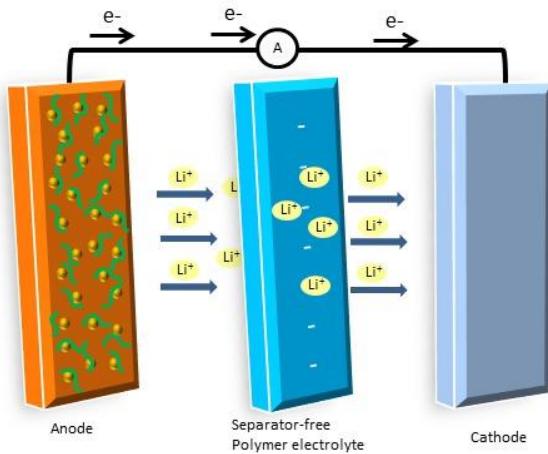


Synthetic polymers with unconventional architectures for energy storage

Pengfei Cao², caopengfei686@gmail.com, Alexei P. Sokolov¹, Tomonori Saito². (1) Chemistry, University of Tennessee, Knoxville, Tennessee, United States (2) Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States

Developing sustainable energy storage technologies has been attracting significant attentions due to the ever-growing energy needs and depleting fossil fuels. Rechargeable lithium ion battery (LIB) has become one of the most successful energy storage devices. Unfortunately, LIBs with common electrolyte still have various problems, such as flammability, toxicity and non-uniform lithium deposition that eventually cause the failure of the cell. Another challenge for energy storage is to improve the energy density of LIB, especially for large-scale applications, such as electric vehicle. Theoretically, using silicon instead of the traditional graphite can raise the capacity up to ten times higher, while the significant volume change during lithiation and delithiation seriously limits the long cycle life of the silicon anode. Developing the high-performance binder can potentially resolve this problem. In this project, we are targeting the development of polymer electrolyte and polymer binders for energy storage applications and study the architecture-property-performance relationship.

For polymer electrolytes, a star-shaped single lithium-ion conducting polymer electrolyte was synthesized by combining the “grafting to” and “grafting from” strategy utilizing a polyhedral oligomeric silsesquioxane (POSS) nanoparticle as the core. The synthesized star-shaped SCPE- Li^+ are characterized by ^1H NMR, FT-IR, UV-Vis, DLS, GPC and DSC, and their ionic conductivity is studied by broadband dielectric spectroscopy. The obtained results reveal a significant “decoupling” of ion conductivity from segmental dynamics for all of the studied SCPE- Li^+ . For polymer binder of anode, we developed a multi-grafting block polymer chitosan-*g*-LiPAA with chitosan as the backbone and lithium polyacrylate as side chains. The architecture effect of multi-grafting copolymer was systematically studied by the galvanostatic test of the assembled coin-type half cells, such as multi-grafting architecture *vs* linear analogue, grafting density and side chain length.



Polymer binder and polymer electrolyte for Li-ion battery

Self-softening shape memory polymers as a substrate for bioelectronic devices

Melanie Ecker, *melanie.ecker@utdallas.edu*. The University of Texas at Dallas, Richardson, Texas, United States

A new generation of materials for neural recording electrodes comprises shape memory polymers (SMPs). These materials have the capability to undergo softening after insertion in the body, and therefore reduce the mismatch in modulus that usually exists between the device and the tissue. We want to understand how a key material property, stiffness, influences the robustness of implantable neuroprosthetic technology. Therefore, we have developed novel intracortical probes which differ only by their ability to soften and become compliant at physiological conditions.

We have applied a new testing protocol to provide accurate thermomechanical measurements of thin SMP films and demonstrate variable compositions to reliably adjust the glass transition temperature (T_g) from 40 to 90 °C in the dry state. Furthermore, we tested test devices in aqueous environments and found that T_g shifts by approximately 10 to 15 °C after plasticization of thin films. Depending on the monomer composition, the polymers could undergo various degrees of softening under physiological conditions, ranging non-softening to softening over 2 magnitudes of order.

Important for the applicability of self-softening, SMP based devices *in vivo* is, that they can be sterilized without altering their thermomechanical properties. Hence, we have studied the response of our SMPs to various sterilization methods listed in the FDA guidance for industry. We have found, that the sterilization with ethylene oxide is an appropriate method for our temperature sensitive polymers.

To get a better understanding of the robustness of the devices, we are currently studying the mechanical durability of the base material and the electrochemical integrity of test devices against accelerated aging in physiological solution at elevated temperatures.

For my future career, I want to focus my research on the enteric nervous system (ENS). Many gastrointestinal diseases are related to dysfunctions of the ENS, but they are not well understood. I want to use my expertise in structure-property relationships of polymers and my knowledge about neural devices, to develop conformal electrode arrays for recording and stimulation of the gut.

Balancing strength and ductility in biomimetic adhesives through breakable bonds

Michael G. Mazzotta, *mmazzott@purdue.edu*, **Michael A. North**, **Amelia A. Putnam**, **Jonathan J. Wilker**. Chemistry, Purdue University, Lafayette, Indiana, United States

Our currently available adhesives tend to be either ductile or strong. Ductility is important to provide a means of distributing out mechanical stresses across the entirety of a bond, instead of concentrating at the edges. Such stress distribution prevents sudden bond failure. However, this property comes at the expense of material strength. Herein, a biomimetic copolymer system was synthesized with a fixed amount of AA and dopamine methacrylamide and toughened with the addition of diols. Incorporation of the acrylic acid monomer provided breakable bonds that promote hydrogen bonding between ethylene glycol molecules and thus induces ductility into the system. The adhesive monomer employed was dopamine methacrylamide representing the DOPA of mussel proteins. While the polymer alone exhibited brittle fracture, incorporation of ethylene glycol results in a brittle to ductile transition, and enhances the strength of the material substantially. This represents a rare example of a biocompatible, wet-setting, flexible adhesive for biomedical applications.

AEI 86

Harnessing the power of post-translational modifications for materials science and engineering

Davoud Mozhdehi, *dmozhdeh@uci.edu*. Biomedical Engineering, Duke University, Durham, North Carolina, United States

Recombinant expression of proteins has emerged as a powerful strategy to access “precision polymers”, offering superb control over the sequence and the length of the final product. However, the precision offered by these recombinant methods is partially offset by the limited repertoire of monomers (canonical amino acids) and linkage chemistry (amide bond). Biology has overcome this limitation ingeniously by modifying proteins after expression using a diverse set of chemical transformations, post-translational modifications (PTMs). PTMs can significantly alter the function, localization and assembly of proteins in biological systems. Additionally, PTMs can be used to decorate proteins with diverse chemical moieties thus expanding the chemical and structural diversity of protein-based materials. Despite these obvious benefits, materials science and engineering community has not fully utilized the power of these diverse modifications to create new hybrid biomaterial.

As a proof of concept, we have recently demonstrated that it is possible to produce precise and well-defined hybrid lipid-protein conjugates, Fatty Acid Modified Elastin-like polypeptides (FAME), in *E. coli* using a simple one-pot expression system. In this presentation, I discuss our progress toward expanding these modifications to more complex lipids such as sterols. These new hybrid biomaterials are thermally responsive and exhibit temperature-triggered hierarchical self-assembly across multiple length scales with varied structure and material properties that can be tuned at the sequence level.

Engineering hierarchical and functional structures with an elegant tool: Polypeptides

Cornelia Rosu, *cornelia.rosu@mse.gatech.edu*. School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia, United States

Nature uses the incredible power of self-assembly to build various structures from simple building blocks (e.g. proteins). Proteins are natural polymers that self-assemble in a programmable fashion at nano- and macro-scales that enable living bodies to efficiently function. It is challenging to develop a complete understanding of this phenomenon because the systems are too complex. By mimicking the biological self-assembly in a synthetic system one can tap into its power and understand how the process works. The advantage of using synthetic systems consists in their simplicity and potential to exhibit properties similar to those of natural homologs. Biopolymers such as polypeptides are the elegant tools to address the above underlined issues. Polypeptides, beside their resemblance to natural proteins, are feasible and sustainable sources to designing benign materials with tunable physical properties.

My research plan will combine fundamental and applied perspectives to discover and manipulate the basic behavior of synthetic systems relevant for applications based on biopolymer self-assembly. In one direction of the studies we will investigate the polypeptide and polypeptide composite particles self-assembly at nano- and macroscale. For practical applications, tailoring the number and length of the amino acid sequences that form a hetero-polypeptide will allow deciphering how the structure-property relationship can be used to process sustainable materials. The second effort in my lab will use polypeptide self-assembly as a tool to organize functional polymers. The results will be applied to understand how polypeptides as bioderived components offer a sustainable route to green processing of semiconducting polymers. The resulting responsive materials will find applications in bioelectronics, wearable/implantable devices and monitoring of food quality. Finally, a third approach in my lab will investigate the self-assembly and self-organization of colloidal cholesteric liquid crystals into nano- and micro-scale hierarchical structures. For practical applications these results will enable the design of complex fluids with tunable properties for optical devices.

Complex fluids and anisotropic liquids for intelligent molecular engineering and material design: Structure-rheology-property relationships

Monirosadat S. Sadati, sansadat@gmail.com. Institute for Molecular Engineering, Chicago, Illinois, United States

I received my PhD degree in Polymer Physics at the *ETH*, in Zürich, under the supervision of Prof. Hans Christian Oettinger. As a PhD student, I worked on various aspects of complex fluids involving the interplay between mesoscale structure and dynamics. I designed a novel experiment, in which a lubricated cross-slot channel was employed to deform polymeric molecules in a complex flow geometry, thereby producing some of the most precise data on the rheology of polymer melts in a mixed shear and extensional flow. In addition, I developed a finite-element based data analysis technique to reconstruct accurate field kinematics from experimental data to examine the performance of rheological models using numerical simulations.

As a postdoctoral fellow in Prof. Fredberg's lab at *Harvard*, I extended the rheology of polymers to biological systems and developed an assay to study dynamics of living cells under geometrical confinement and designed a new device to explore intercellular shear deformation.

In my current postdoctoral position at the *University of Chicago*, I work on structural organization and potential applications of liquid crystalline materials under the supervision of Prof. Juan de Pablo. I have shown that liquid crystal-aqueous interface is capable of reporting aggregation of polypeptides at early stages and reducing water activity by adding salts to the aqueous phase can initiate transport of dissolved water in the liquid crystal phase. These results provide fundamental principles for designing biological sensors, drug delivery systems, and molecular machines. Furthermore, working with scientists at the Argonne National Laboratory, we have obtained structural information of liquid crystal molecules at the interfaces using synchrotron X-ray reflectivity and Grazing-incidence small-angle scattering measurements.

As a new faculty member, my future research will include exploring structure-rheology-property relationships of polymeric materials and lyotropic liquid crystalline mesophases, focusing on linking molecular to micron scale phenomena and finding new routes to engineer new functional materials with tunable properties for drug delivery, biomedical and photonics applications. Moreover, building on my background in polymer physics and harnessing my expertise in characterization techniques, I have a particular interest in understanding the rheological and processing aspects of additive manufacturing to develop strategies for materials optimization.

Understanding marine bio-adhesion: Characterization of the eastern oyster cement

Andres M. Tibabuzo³, atibabuz@purdue.edu, Erik Alberts², Stephen Taylor⁴, Jonathan J. Wilker¹. (1) Purdue Univ, West Lafayette, Indiana, United States (2) Purdue University, West Lafayette, Indiana, United States (3) Chemistry, Purdue University, West Lafayette, Indiana, United States

Biological systems have been the inspiration of mankind in the development of new tools and technologies as well as a vast array of materials used in our daily life. From the silk in our shirts, the leather and rubber in our shoes to the glue that we use to stick them together almost all of it can be traced back to a biological system. Of these systems, oysters are an interesting example. Through evolution oysters have found a solution to endure the challenges of living in an environment that is constantly changing. One of the solutions is the development of adhesives that are able to maintain their structural integrity on wet and dry conditions. Being a commercially important organism, the eastern oyster (*Crassostrea virginica*), has been studied mainly in the context of breeding, for production in fisheries, and for the ecological role that they play filtering the water of estuaries. However, little to almost no attention has been directed toward the study of the biomaterial they produce to attach themselves to a substrate. Due to the limited amount of information on the adhesive properties of oyster cement and the ever-increasing need for new materials we present in this study a first approach to the characterization of this biomaterial, using a wide array of techniques from microscopy to proteomics, in larval and adult stages of the eastern oyster.

Programming self-assembly and function at multiple scales with nucleic acids

Jeffrey Vieregg, jvieregg@uchicago.edu. Institute for Molecular Engineering, University of Chicago, Chicago, Illinois, United States

Control of molecular structure and reactivity at the nanometer scale has been a dream of chemists for years. For far longer, Nature has accomplished this feat with immense variation and scale, relying on bottom-up self-assembly of genetically evolved components to build structures and reaction pathways far more complex than anything humans can design. Nucleic acid nanotechnology has emerged as an exciting field in which the programmable hybridization rules of Watson-Crick base pairing are used to construct intricate two- and three-dimensional structures, carry out logic operations, and build molecular circuits and motors that operate at the smallest of scales. The theme of my proposed research is to leverage the advances of nucleic acid nanotechnology to build *functional* nano-devices capable of carrying out chemical transformations and probing biochemical systems *in vitro* and *in vivo*.

Programming chemical reactivity

I have recently developed new methods to form site-specific covalent linkages between oligonucleotides and proteins, and plan to use these to design enzymatic cascades in which the product of one reaction immediately becomes the substrate of another, avoiding the need for high intermediate concentrations. Additionally, I will continue a collaboration developing nucleic acids as conformationally-controllable ligands for organometallic catalysis.

Biomolecular phase transitions

In both membraneless organelles and pathological aggregates, molecular conformation change drives phase separation *in vivo*. We recently found that the phase of nucleic acid-peptide complexes is controlled by nucleic acid hybridization. I plan to extend this work to full-length mRNA and proteins in order to determine the physical principles governing phase transitions in normal and pathological states. The same principles will enable the design of nanoparticles for more efficient delivery of therapeutic nucleic acids, a key challenge to realizing the potential of therapies such as siRNA.

Nucleic acid nanotechnology *in vivo*

Despite their inherent biocompatibility and therapeutic potential, the vast majority of nucleic acid nanodevices function only in test tubes. Building upon the outcomes of the above projects, as well as studies I am currently pursuing on the effect of crowding on strand displacement dynamics, I plan to develop nucleic acid nanodevices capable of sensing genetic state and producing therapeutic products when and where they are needed, in living organisms.

Three-dimensional responsive soft micro/nano-structures for biomedical and electronic applications

Weinan Xu, *weinanxu@gmail.com*, **David H. Gracias**. Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, Maryland, United States

Responsive soft micro/nanostructures have attracted much attention in recent years due to their abilities to adapt and respond to external stimuli, and promising applications in biosensing, drug delivery, self-healing materials and flexible electronics. To further improve the performance of the 3D responsive structures, novel and smart materials need to be used as the building blocks. In this work, novel polymers with branched architecture and multi-responsive properties were used to fabricate hierarchical microcapsules, which have the ability to simultaneously encapsulate multiple types of cargo molecules, and release them in a programmable manner triggered by external stimuli. On the other hand, for the fabrication of 3D bioelectronics, 2D nanomaterials including graphene and transition metal dichalcogenides, were utilized as the major component. The 2D materials were folded into well-defined 3D geometries by combining surface functionalization and top-down fabrication. Such 3D graphene microstructures have the ability to encapsulate biological samples such as live cells, which enables highly sensitive 3D analysis, mapping and sensing. To sum up, responsive 3D soft micro/nano-structures were built with novel and smart components, which leads to hierarchical internal structures and superior performance compared with traditional ones, such ultra-thin, flexible, and biocompatible 3D structures provide a new platform for bioelectronics, biosensing and drug delivery.