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| 39       | Lucas, H.             | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 40       | O'Connor, M.          | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 41       | Remy, M.              | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 42       | Roering, A.           | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 43       | Sears, R. B.          | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 44       | Strausberg, L.        | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 45       | Garcia Sega, E.       | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 46       | Ogbomo, S.            | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 47       | Bizier, N.            | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 48       | Desmond, R.           | ●    | ●   |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 49       | Fisher, E.            | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 50       | Hahn, J.              | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 51       | Haynes, D.            | ●    | ●   | ●   |     |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 52       | Kesharwani, T.        | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 53       | Mallia, A.            | ●    | ●   | ●   |     |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 54       | Niskala, J.           | ●    | ●   | ●   |     |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 55       | Patil, A.             | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 56       | Van Dyke, A.          | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 57       | Chapman, C.           | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 58       | Keasler, S.           | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 59       | Kulik, H.             | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 60       | Milojevich, C.        | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 61       | Sivak, D.             | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 62       | Steeves, A.           | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 63       | Velarde, L.           | ●    | ●   | ●   |     |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 64       | Ball, N.              | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 65       | Kota, A.              | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 66       | Marpu, S.B.           | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 67       | Singh, V.             | ●    | ●   |     |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 68       | Singh, Y.             | ●    | ●   |     |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 69       | Uribe-Romo, F.        | ●    | ●   |     |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 70       | Cheung-Lau, J.        |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 71       | Milligan, K.          | ●    |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
| 72       | Zhao, L.              | ●    | ●   |     |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |

*Poster numbers may change due to late withdrawals
1. **Elizabeth Crew**, Department of Chemistry, Binghamton University, Binghamton, NY 13902. ecrew1@binghamton.edu; Binghamton University, State University of New York (B.A., 2001; M.S., 2005; Ph.D. anticipated 2013), Dr. Chuan-Jian Zhong (Chem), Nanoprobe transduction in biomolecular detection for cancer diagnostics.

My aims and goals for employment in the academic field are multifaceted. I truly love to teach, especially analytical chemistry. My research interests include the use of surface engineered nanoparticles in biomedical and green chemistry applications. I would like to encourage more women to enter the field of chemistry and to introduce them to the research environment, since women are underrepresented in scientific fields. I would prefer to teach at a four-year institution, as I wish to focus on teaching, but I would be willing to work at a graduate-level institution as well.

Abstract Title: *Engineered nanoparticles for biomedical analysis*

ANYL, COLL Divisions

2. **Dipankar Koley**, Department of Chemistry, University of Michigan, Ann Arbor, MI 48109-1055. dkoley@umich.edu; Haldia Institute of Technology, West Bengal, India (B.Tech, Hons., 2003); Texas A&M Commerce (M.S., 2005); The University of Texas at Austin (Ph.D., 2011), Dr. Allen J. Bard, Application of scanning electrochemical microscopy (SECM) in biological systems; Postdoctoral Researcher at The University of Michigan at Ann Arbor (2011–present), Dr. Mark E. Meyerhoff, Electromodulated NO release from inorganic nitrite salts for potential use as an anti-coagulant as well as anti-microbial agent to prevent biofilm formation on catheter surfaces.

My research program will primarily focus on developing a new set of electrochemical techniques to study complex biological systems with special interest in the area of microbial biofilms. Initial fundamental understanding of these biological systems will then be used to design next-generation biomedical devices such as implantable sensors, catheters, and other devices. I have assisted in teaching graduate-level electrochemistry courses as well as undergraduate labs and hope to continue at a graduate-level institution.

Abstract Title: *Applications of electrochemical techniques to study biological…*

ANYL, BIOL Divisions
3. **Eric J. Dimise**, Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, 240 Longwood Ave., Building C1-609, Boston, MA 02115. Eric_Dimise@hms.harvard.edu; 617-432-3801; Union College (B.S., 2005); Boston College (Ph.D., 2010), Dr. Steven D. Bruner (Chem), The discovery, isolation, structure elucidation, and total synthesis of the Fuscachelins, nonribosomal peptide siderophores from the thermophilic actinomycete *Thermobifida fusca*; Postdoctoral Researcher at Harvard Medical School (2010–present), Dr. Jon Clardy, Isolation, structure elucidation, and biological assay of small molecules that induce growth of uncultured microbes.

I am seeking a position at a four-year college that strongly emphasizes excellence in undergraduate education. I have taught undergraduate lab sections in organic chemistry and instrumentation and have mentored undergraduate researchers. I have assisted in teaching graduate-level courses that focused on current topics in biological chemistry, which included writing and giving lectures. My research will focus on small-molecule natural products that impact growth and development in environmental microbes. The tools of organic synthesis and structure elucidation (i.e. NMR, MS) will be used to probe the chemical basis of these important biological phenomena.

Abstract Title: **Small molecule natural products enable microbial growth**

BIOL Division

4. **Elisha N. Fielding**, Center for Marine Biotechnology and Biomedicine, Scripps Institution of Oceanography, University of California San Diego, 8655 Kennel Way, La Jolla, CA 92037-0204. efielding@ucsd.edu; University of Tennessee at Chattanooga (B.S., Chem, 2003); Boston College (Ph.D., Chem, 2010), Prof. Steven Bruner, Substrate recognition and catalysis by DpgC, a cofactor-free dioxygenase in vancomycin biosynthesis; Postdoctoral Scholar at Scripps Institution of Oceanography, UCSD (2010–present), Prof. Bradley Moore, Biosynthesis of marine microbial natural products.

My research uses an interdisciplinary approach and techniques from the fields of synthetic chemistry, biochemistry, and structural and molecular biology to understand how microbes assemble bioactive small molecules. I have been a teaching assistant for labs and lectures for typical undergraduate chemistry majors’ courses (General, Organic, Biochemistry); for Physical Chemistry for Biochemistry Majors and Frontiers in Life Science (a general course for nonscience majors); and for a graduate-level Enzyme Mechanisms course. I have supervised the research of four undergraduates, one of whom wrote a senior honors thesis based on their research.

Abstract Title: **Natural and nonproteogenic amino acids in natural product...**

BIOL Division
5. Kathleen C. A. Garber, Department of Chemistry, Indiana University, Simon Hall, 212 S. Hawthorne Drive, Bloomington, IN, 47405. garber@indiana.edu; 812-856-9948; Franklin & Marshall College (B.A., 2003); University of Wisconsin–Madison (Ph.D., 2010), Professor Laura Kiessling, A general glycomimetic scaffold yields probes to explore C-type lectin function; Postdoctoral Fellow at Indiana University (2011–present), Professor Erin Carlson, Chemical tools for the selective detection of phosphorylated proteins.

I am seeking a faculty position at a research-intensive, primarily undergraduate institution. As a faculty member, I plan to develop an interdisciplinary research program focusing on the discovery, bioactivity, and synthesis of natural products. Additionally, I am eager to use my experience mentoring undergraduates both in the classroom and the laboratory. I am interested in teaching typical undergraduate courses, such as biochemistry and organic chemistry. Additionally, I would like to establish upper-level courses and laboratories that require students to draw on their previous coursework to develop the concepts and tools needed to contribute to the field of natural product discovery.

Abstract Title: Chemical tools for the selective detection of phosphorylated proteins

BIOL, ORGN Divisions

6. Christopher J. MacNevin, Department of Pharmacology, and Center for Integrative Chemical Biology and Drug Discovery, University of North Carolina at Chapel Hill, Genetic Medicine Building, Room 4009, 120 Mason Farm Road, Chapel Hill, NC 27599. cmacnev@med.unc.edu; 404-538-3386; Trinity College, Hartford, CT (B.A., Psych, 1994); University of North Carolina at Wilmington (M.S., Chem, 2003); Emory University (Ph.D., Chem, 2008), Dr. Dennis Liotta, Stereoselective synthesis of quaternary center bearing azetines and β-amino acids; Natural and enantiomeric progesterone derivatives for the treatment of traumatic brain injury; Postdoctoral American Cancer Society Research Fellow at University of North Carolina at Chapel Hill (2009–present), Dr. Klaus Hahn and Dr. Stephen Frye, In vivo protein labeling and biosensor applications using environment-sensing fluorophores.

My research interests focus on designing and applying chemical tools to probe biology, with specific focus on epigenetic processes related to cancer and aging. I seek a faculty position at a primarily undergraduate four-year college or university, where I intend to lead a research program that gives students experience in chemical biology. I am interested in progressive teaching methods that maximize student engagement and the development of critical thinking skills. My teaching experience includes over three years of leading organic and general chemistry laboratory courses, as well as mentoring undergraduate and graduate students in advanced research projects.

Abstract Title: Building better biosensors with the tools of chemical biology

ORGN, BIOL, MEDI Divisions
7. **Paul A. Vadola**, Department of Chemistry and Molecular Pharmacology, Memorial Sloan Kettering Cancer Center, New York, NY 10065. vadolap@mskcc.org; 917-593-6429; Fordham University (B.A., 2004); Columbia University (M.S., 2007; M.Phil., 2009; Ph.D., 2010), Prof. Dalibor Sames, C–H Bonds as ubiquitous functionality: New methods for the activation and functionalization of C–H bonds; NIH Ruth Kischstein Postdoctoral Fellow at Memorial Sloan Kettering Cancer Center (2010–present), Prof. Samuel J. Danishefsky, The chemical syntheses of fully glycosylated homogeneous human chorionic gonadotropin and human luteinizing hormone.

I am seeking a faculty position at a college or small university. As a professor, my primary goal is to impart a strong understanding of fundamental scientific concepts, to both science majors and nonmajors, in order to build critical thinking skills and an appreciation for the physical sciences. I have experience as an adjunct faculty member teaching a nonmajors physical science course and my graduate and postdoctoral research has prepared me to teach courses in organic, inorganic, and biochemistry. My research plan has been designed with undergraduates in mind and will serve to reinforce the concepts discussed in the classroom.

Abstract Title: *Progress toward the chemical synthesis of human chorionic…*

ORGN, INOR, MEDI Divisions

8. **Mangalika Warthaka**, College of Pharmacy, University of Texas at Austin, 107 West Dean Keaton, Biomedical Engineering Building, Austin TX 78712-0165. mangalar@mail.utexas.edu; University of Kelaniya, Sri Lanka, (B.Sc., Hons, 1996); Wayne State University (Ph.D., 2007), Dr. Mary May Pflum, Development of proteomic tools for monitoring peptide and protein phosphorylation; Postdoctoral Fellow at University of Texas at Austin (2008–2011), Dr. Kevin N. Dalby, Structural and mechanistic studies of ERK2: Ets-1 complex; Postdoctoral Fellow at Texas Screening Alliance for Cancer Therapeutics (2011–present), [Name of professor not provided], Development of ERK2 inhibitors and assays for screening potential therapeutic targets.

Understanding protein–protein interactions and the mechanism of actions in ubiquitination mediated kinase activation will be my continuing research interest. In addition, I am interested in developing small molecule and peptidomimetic inhibitors to disrupt these protein–protein interactions. As an instructor, I would like to use my organic chemistry quiz and laboratory teaching experience and pursue teaching in organic chemistry and biochemistry graduate and undergraduate classes. I like to focus both on research and teaching and prefer research-oriented universities either with Ph.D. or master’s degree programs.

Abstract Title: *Delineating MAPK-substrates interactions using molecular…*

ORGN, BIOL, MEDI Divisions
9. Benjamin J. Wylie, Department of Chemistry, Columbia University, 3000 Broadway Havemeyer Hall, MC 3132, New York, NY 10027. bw2276@columbia.edu; The College of William and Mary (B.S., Chem, 1998); University of Illinois at Urbana-Champaign (Ph.D., Chem, 2008), Dr. Chad M. Rienstra, Solid-state magic-angle spinning NMR methods for tensor measurements and protein structure refinement using chemical shift tensors; NIH NRSA Postdoctoral Fellow (2008–present), Dr. Ann E. McDermott, Structure and characterization of integral membrane proteins using three- and four-dimensional solid-state NMR (SSNMR) and dynamic nuclear polarization (DNP).

I plan to use SSNMR to characterize and solve the structures of membrane proteins and large oligomeric systems. My past research established new benchmarks for structural precision and resolution obtainable by SSNMR, and I plan to extend this capability. In graduate school I accrued significant teaching experience, including both graduate and undergraduate classes. I have also taught several laboratory courses, beginning as an undergraduate student. As a graduate student and postdoctoral fellow, I have mentored several undergraduate researchers and graduate students in the early stages of their research. I want to teach and direct research at a research university.

Abstract Title: *New adventures in structural biology via solid-state NMR*

BIOL, PHYS Divisions

10. Anirudha Singh, No biographical sketch provided

Abstract Title: *Multifunctional biomaterials using nanobeads*
I am seeking a faculty position at a primarily undergraduate institution, a teaching-track position at a Ph.D.-granting institution, or a tenure-track position in chemistry education research. I look forward to teaching introductory chemistry, physical chemistry, and computational chemistry. I plan to continue my research in chemistry education with collaborators in education psychology and learning science, focusing on educational simulations, educational games, and online curriculum. As a TA for both undergraduate and graduate students at MIT, I developed a passion for challenging and equipping students and I look forward to further opportunities to teach, inspire, and mentor them.

Abstract Title: *Advancing chemistry and interdisciplinary STEM education…*
12. Michael A. Bruckman, Biomedical Engineering, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, OH 44106. Michael.bruckman@case.edu; SUNY University at Buffalo (B.A., Chem, 2004), Dr. Bing Gong, Synthesis and characterization of novel helical foldamers with a partial positive interior channel; University of South Carolina (Ph.D., 2009), Dr. Qian Wang, Tobacco mosaic virus as a scaffold for cell adhesion, nanoelectronics, and VOC sensing; Postdoctoral Fellow at Naval Research Laboratory (2009–2011) Dr. Banahalli Ratna, Self-assembly of nano split ring resonators with tobacco mosaic virus as a template; Postdoctoral Researcher at Case Western Reserve University (2011–present) Dr. Nicole F. Steinmetz, Engineering rod-shaped viral nanoparticles for a magnetic resonance imaging–based theranostic platform for treatment of cardiovascular disease.

My primary goal is obtaining a tenure-track research faculty position at a university. I seek to build an interdisciplinary research program focusing on developing viral nanoparticles as a platform technology in fields ranging from sensing and energy to biomedicine. Teaching and mentoring students through these fields presents interesting challenges relating to multidisciplinary requirements and cutting edge research. I plan to incorporate multidisciplinary coursework into my program. My publication record demonstrates focus, extraordinary productivity, creativity, and vision. I always strive to continue my education via pursuing research in new, exciting fields of science by integrating viral nanoparticles for developing novel materials.

Abstract Title: Development of a viral nanoparticle for biomedical applications

COLL, PMSE Divisions

13. Shelley A. Claridge, California NanoSystems Institute and Department of Chemistry and Biochemistry, University of California, Los Angeles, Los Angeles, CA 90095. claridge@cnsi.ucla.edu; [Undergraduate degree and institution unknown]; University of California, Berkeley (Ph.D., 2008), Prof. A. Paul Alivisatos and Prof. Jean M. J. Fréchet, Inorganic nanocrystal bioconjugates: Asymmetry, proximity, and enzymatic manipulation; NIH Postdoctoral Fellow, UCLA (2009–present), Prof. Paul S. Weiss, Microwave-modulated scanning tunneling microscopy of peptide structure.

My research interests lie in two complementary directions: 1) Using biology to control nanomaterial assembly for plasmonic and sensing applications. 2) Using nanoscience to understand biological structure and function via nanocrystal bioconjugates and physical techniques such as scanning tunneling microscopy. My goal is to establish a strong research program at a Ph.D.-granting institution. As a graduate student at Berkeley, I received three teaching awards for freshman honors and sophomore organic chemistry and took a leadership role in graduate recruiting for the department. At UCLA I have served as President of the Society of Postdoctoral Scholars for the past two years.

Abstract Title: Understanding and controlling biological structure and…

COLL, PHYS Divisions
14. Preston B. Landon, Department of Bioengineering, Department of Mechanical and Aerospace Engineering, The University of California, San Diego, 9500 Gilman Drive M/C 0411, La Jolla, CA 92093. Plandon@ucsd.edu; 858-754-7609; University of La Verne (B.S., Physics, 1997); University of Texas at Dallas (Ph.D., Physics, 2005), Dr. Robert Glosser, Nano-engineering of colloidal particles, synthetic biomimetic blood cells, synthetic opals, photonic crystals, and the physics of self-assembling nanostructures; Postdoctoral Researcher at the University of Chicago, Department of Medicine, Center for Nanomedicine, (2007–2009), Dr. Ratnesh Lal, DNA zippers and springs, telomerase specific DNA zippers; Postdoctoral Researcher at The University of California, San Diego, Department of Mechanical and Aerospace Engineering, Department of Bioengineering, (Jan. 2010–present), Dr. Ratnesh Lal, Smart drugs.

My research currently focuses on creating a colloidal particle that opens upon detecting a specific mRNA. I have publications demonstrating my experience with the optical properties and fabrication of photonic crystals, self-assembly of colloidal silica into synthetic opals, colloidal particle synthesis, and functional DNA-based devices. I am seeking a faculty position where I can teach classes and pursue research. While completing my doctoral research, I independently advised, mentored, and created research projects for undergraduate students, 10 of whom I included as authors in resulting publications. A student I worked with was awarded the NSF Graduate Research Fellowship.

Abstract Title: Colloidal particle synthesis, DNA zipper based springs, and drug...

COLL, PMSE, MEDI Divisions

15. Dhriti Nepal, No biographical sketch provided

Abstract Title: Design, synthesis, and assembly of nanoscale building blocks for...
16. Rosalynn Quiñones, Department of Chemistry, Washington & Jefferson College, 60 South Lincoln Street, Washington, PA 15301. rquinones@washjeff.edu; University of Puerto Rico (B.S., 2003); Duquesne University (Ph.D., 2008), Dr. Ellen S. Gawalt (Chem), Modification of nitinol, nickel, and titanium oxides with self-assembled monolayers, and polymers for corrosion mitigation in biomaterial applications; AGEP Postdoctoral Research Associate at University of Michigan (2008–2010), Dr. Adam J. Matzger (Chem), Discovery and screening of new crystal forms (polymorphism) of pharmaceutical compounds; NSF Postdoctoral Research Fellow (2011–present), Dr. Robbie Iuliucci (Chem), Polymer brushes created by surface modified metal oxide nanoparticles with organic acids and their characterization using NMR.

I seek a faculty position at a primarily undergraduate institution where excellence in teaching as well as student research is valued. My research focus (surface and colloid functionalization using thin films) has granted me extensive knowledge of analytical characterization using spectroscopy, thermal analysis, and electrochemical methods. In addition to previously teaching general chemistry lab and recitation, and analytical and organic lab, I have designed an advanced instrumental lecture and lab course. I also value interdisciplinary learning and am developing a laboratory travel course (January 2013) for both science and nonscience majors that explores the wonders of science in Puerto Rico.

Abstract Title: Controlling surface properties of metal oxide nanoparticles using…

COLL, ANYL, POLY Divisions
17. Jefferson E. Bates, Chemistry Department, University of California, Irvine, 1102 Natural Sciences II, Irvine, CA 92617. batesj@uci.edu; The College of William and Mary (B.S., 2008); University of California, Irvine (Ph.D., anticipated June 2013), Dr. Filipp Furche, Systematic improvements of density functionals and new divalent lanthanide chemistry; Pedagogical Fellow at University of California, Irvine (2011–2012).

My research interests focus on the application of electronic structure methods to the design and characterization of inorganic compounds for artificial photosynthesis and future energy sources. I am interested in developing novel methods and algorithms that accurately describe noncovalent interactions to study molecular catalysis in conjunction with experimental groups. Building on my experience as a Pedagogical Fellow and K–12 outreach tutor, I am committed to creating a student-centered learning environment and making chemistry accessible to a broad audience through visualization and analogy. I plan to build an externally funded research group for students and postdocs at a research university.

Abstract Title: *Computational studies of unexpected 5d rare-earth metal reduction…*

COMP, PHYS Divisions

18. Dinadayalane Tandabany, Interdisciplinary Center for Nanotoxicity, Department of Chemistry and Biochemistry, Jackson State University, Jackson, MS 39217. dina@icnanotox.org; 601-212-6748; Pondicherry University, India (B.S., 1998; M.S., 2000); Pondicherry University, India (Ph.D., 2005), Dr. G. Narahari Sastry, A theoretical study on the structural, energetic, and reactivity aspects of model organic compounds; Postdoctoral Research Associate at Jackson State University (2005–present), Prof. Jerzy Leszczynski, High-performance computational investigations of Stone-Wales defects and reactivity in single-walled carbon nanotubes: Applications toward hydrogen storage and sensors.

Publications: 40 articles, 6 book chapters. $h$ index—14.

I seek a faculty position to establish externally funded research programs and mentor students. Research interests: applying computational methods to understand structures, properties, and reactivities of novel hybrid nanomaterials. Teaching experience: both graduate and undergraduate levels—general chemistry, quantum chemistry, and atomic and molecular spectroscopy. I have been involved in writing proposals, some of which were funded in the last six years. I have been supervising graduate (Ph.D.) and undergraduate students since 2006. I would very much like to teach and mentor students in research at a regional university.

Abstract Title: *High performance computational investigations of Stone-Wales…*

COMP, PHYS, ORGN Divisions
19. **Igor Leontyev**, Department of Chemistry, University of California, Davis, One Shields Avenue, Davis, CA 95616. ileontyev@ucdavis.edu; Moscow Engineering Physics Institute (B.S., 1999); Karpov Institute of Physical Chemistry (Ph.D., 2004), Prof. M. Basilevsky (PChem), Molecular mechanisms of equilibrium/nonequilibrium solvation effects; Postdoctoral Research Fellow at National Institute of Advanced Industrial Science and Technology, Japan (2004–2005), Prof. M. Tachiya (PChem), Polarizable MD simulation of electron transfer reactions; Postdoctoral Research Fellow at University of California, Davis (2006–present), Prof. A. Stuchebrukhov (Bio), Computer simulation of central enzymes of cellular energy generating system.

My expertise is in the development and application of computational tools to chemical and biophysical problems. A study of theoretical methods and their improvement can be an excellent subject for student research, serving as teaching material with high scientific potential. I have been mentoring graduate and undergraduate students for the past six years. My academic background provided extensive experience in presenting material and using modern visualization tools to enhance comprehension of difficult concepts. I would like to teach and direct student research at all levels (undergraduate through Ph.D.) at a higher education and research institution.

Abstract Title: *New approach to biological simulations*

COMP, PHYS, BIOL Divisions

20. **Tyler Luchko**, BioMaPS Institute, Rutgers University, 174 Frelinghuysen Road, Piscataway, NJ 08854-8087. tluchko@rutgers.edu; University of Alberta (B.Sc., 2000; Ph.D., 2008), Prof. Jack A Tuszynski (Physics) and Dr. Andriy Kovalenko (National Institute for Nanotechnology, Mech Eng) Molecular modeling of protein–protein/protein solvent interactions; Postdoctoral Associate at Rutgers University (2009–present), Prof. David A. Case, Integral equation theory of biomolecule solvation.

My interests lie in the use of statistical mechanics and computational methods to model biomolecules and understand the role of solvation. Recent work focuses on the ionic atmosphere of DNA and water-mediated protein–ligand binding. I am currently working with graduate students to develop these methods and, as a graduate student, I assisted with and helped to develop two undergraduate computational physics courses. I am seeking a teaching and research position where I can work with undergraduate and graduate students at the intersection of chemistry, physics, computation, and biology.

Abstract Title: *Implicit solvent calculations with explicit molecular models in…*

COMP, PHYS, BIOL Divisions
I use theory and computation to understand the physical principles underlying nascent protein behavior in living cells using such tools as physics-based coarse-grained simulations of macro-molecular complexes, such as the ribosome; chemical kinetic modeling; polymer theory; and systems biology methods. Papers in *Nature Communications*, *JACS*, and *PNAS*. Three nationally competitive grants, NSF and NIH. Future research focusing on modeling and predicting properties of nascent chain folding, misfolding, and aggregation using published transcriptome-wide experimental data (such as from ribosome profiling) will directly apply to theoretical chemistry, synthetic biology, biotechnology, and biomedicine. I seek to obtain a tenure-track position at a research-intensive university.

Abstract Title: *In vivo protein biophysics: Insights from novel theoretical and...*

COMP, PHYS, BIOL Divisions

22. Eduardo Sproviero, No biographical sketch provided

Abstract Title: *Development and application of computational methods to biological...*
23. Sinisa Vukovic, Oak Ridge National Laboratory, MS 6119, Oak Ridge, TN 37831. vukovics@ornl.gov; University of Saskatchewan (B.Sc., Chem, 2001; B.Sc., Math, 2001); University of Toronto (M.Sc., Chem, 2003; Ph.D., Chem, 2007), Prof. R. A. McClelland, I. Molecular mechanism of GPCRs, II. Carbocationic polymerization of styrene; Postdoctoral Fellow at the University of Pisa, Italy (2008), Dr. Benedetta Mennucci, Enhanced fluorescence near metal nanoparticles; Postdoctoral Fellow at the University of California, Berkeley (2009) and Lawrence Berkeley National Laboratory (2010), Dr. William A. Lester, Jr., Quantum Monte Carlo; Postdoctoral Fellow at Oak Ridge National Laboratory (2011–2013), Dr. Ben P. Hay, Computer-aided molecular design.

My research focus is on organic reaction mechanisms, molecular design, and applied chemistry curriculum. I am a self-motivated researcher (chose topics for my thesis and all three projects for my postdocs, and obtained super computer time from ESF and DOE). The difference between science (search for truth) and research (search for funding) is clear to me. Since I graduated, I have taught chemistry courses as an Instructor for four semesters (General I, Organic I and II, Computational) and supervised 24 undergraduate students (obtained funding for each student). I seek a position teaching at a Ph.D.-granting institution.

Abstract Title: *From the first principles to design to synthesis to application of...*

COMP, ORGN, PHYS, INOR Divisions
24. Shijun Zhong, Computer-Aided Drug Design Center, School of Pharmacy, University of Maryland, 20 Penn Street, Baltimore, MD 21201. sjzhong@gmail.com; [Undergraduate degree unknown]; Xiamen University (Ph.D., 1994), Qianer Zhang, Simplification of two-electron integral computation using symmetry method or irreducible tensor method; Assistant Researcher at Chinese Academy Fujian Institute, (1994–1996), Chunwan Liu, Theoretical study of fullerenes and cage structures; Associate Professor at Xiamen University (1996–1999); [Candidate is the associate professor], Real irreducible tensorial set; Postdoctoral Fellow at University of California, Berkeley (1999–2000), Teresa Head-Gordon, Fragmentation of molecular electrostatic potential for protein; Postdoctoral Fellow at Wesleyan University in Connecticut, (2000–2003), George Petersson, New generation of Gaussian basis sets for quantum chemistry; Postdoctoral Fellow at University of Maryland (2004–present), Alexander D. MacKerell, Jr., Molecular dynamics simulation of protein and drug design.

I am interested in developing computational methods and applying them to chemical and biological molecules, particularly focusing on the interaction between small compound and protein toward drug design. I hope to interest students in chemistry and biochemistry through this research, via extracting concepts from theoretical analysis and developing protocols for performing molecular modeling toward meaningful information that can be used to explain experimental phenomena. I taught physical chemistry and quantum chemistry courses. I developed a training program in scientific computation. I want to teach and direct the research of undergraduate and graduate students at a four-year institute or comprehensive university.

Abstract Title: Developing methods of computational chemistry and biology

COMP, PHYS Divisions

25. Sushil Kanel, No biographical sketch provided

Abstract Title: Fate and transport of nanoparticles and their applications for soil, water,....
26. Hyun Ji (Julie) Lee, Department of Chemistry, University of California, Irvine, 25 Bower Tree, Irvine CA, 92603. hlee18@uci.edu; California State University, Fullerton (B.S., Chem, 2006); University of California, Irvine (M.S., Chem, 2008; Ph.D., Chem, 2011), Dr. Donald R. Blake (Chem), Breath analysis on patients undergoing hemodialysis (HD) and identification of exogenous and endogenous sources for compounds found in breath; Postdoctoral Researcher at UC Irvine Chemistry Department (2012–present), Dr. Sergey A. Nizkorodov, Creating aged secondary aerosols in a chamber and analyzing them through various forms of spectroscopy (UV-Vis, fluorescence, Raman Spectroscopy, and laser-induced triple state process); Removing browning effects in photo-bleaching aged SOA aerosols.

As an atmospheric specialist and a current member of the Aerosol Photochemistry Group at UC Irvine, I have a track record of conducting insightful research on aerosols and whole-air chemistry. I have been involved in various NASA airborne and ground-based studies, and I have participated in grid, ecological, and bio-analytical research. In my current work, I have been analyzing secondary organic aerosols. I am interested in developing instruments and designing studies to research tropospheric chemistry, aerosols, whole-air chemistry, and aerosol-cloud–climate interactions. I am interested in career opportunities with a national research lab or a four-year college or university.

Abstract Title: Characterizing air mass collected at lower troposphere(< 2km) during...

ENVR, ANYL, COMP Divisions

27. Camille Petit, Departments of Earth and Environmental Engineering and Chemical Engineering, Columbia University, 500 West 120th Street, New York, NY 10027. cp2577@columbia.edu; Ecole Nationale de Chimie de Montpellier, France (B.S., 2005; M.S., 2007); The Graduate School of the City University of New York (Ph.D., Chem, 2011), Prof. Teresa J. Bandosz, Design of reactive carbon-based adsorbents for the gas separation of small molecules; Postdoctoral research at Columbia University (2011–present), Prof. Ah-Hyung Alissa Park, Synthesis, characterization, and evaluation of novel liquid-like nanoscale inorganic–organic hybrid materials for CO2 capture.

My research training covers the areas of materials science, environmental chemistry, and separation processes. Using this expertise (25 peer-reviewed publications), I would like to direct a research program at a four-year college or comprehensive university on the development of novel nanomaterials as a platform to address critical issues of sustainability. I hope to spark the interest of students in this area via both teaching and research. During my graduate and postdoctoral work, I served as a lecturer and teaching assistant for different undergraduate and graduate courses and also mentored students toward the completion of their research studies.

Abstract Title: Nanoscale hybrid materials for sustainability

ENVR, COLL, PMSE Divisions
28. **Jesse G. Thompson**, Center for Applied Energy Research, University of Kentucky, 2540 Research Park Drive, Lexington, KY 40511. jesse.thompson@uky.edu; Western Michigan University (Ph.D., 2011), Dr. John B. Miller, Characterizing potential feedstocks for biofuel production; Postdoctoral Scholar at University of Kentucky (2012–present), Dr. Joe Remias, Investigating the degradation of amine solvents used in post-combustion carbon capture.

I’m currently focusing on identifying and quantifying degradation products from amine-based solvents used in post-combustion carbon capture from coal power plants. My primary interest is developing new sampling techniques for emissions from flue gas stacks and incorporating high-resolution MS to identify and quantify trace amine degradation products formed during the carbon capture process. Previous research: environmental analysis, green chemistry, life-cycle assessments, chemometrics, sensory evaluations, sustainable energy development, and biofuel production from waste materials. I’m interested in developing an externally funded research group at an M.S.- or Ph.D.-granting institution and engaging in educational research in addition to normal teaching duties.

Abstract Title: *Analyzing post combustion CO₂ capture solvent degradation products*

ANYL, ENVR, FUEL Divisions

29. **Yonghong Zou**, Illinois Sustainable Technology Center, University of Illinois Urbana-Champaign, 1 Hazelwood Drive, Champaign, IL 61820. yhzou@illinois.edu; Beijing University of Chemical Technology (B.S., 2001); University of Wisconsin-Milwaukee (M.S., 2009; Ph.D., 2011), Dr. Erik Christensen, PCB and PBDE characteristic sources and degradation pathways in aquatic sediments; Postdoctoral Research Associate at Illinois Sustainable Technology Center, University of Illinois at Urbana-Champaign (2011–present), Dr. Wei Zheng, Colloid-facilitated transport of hormones and antibiotics in agriculture soils.

I am interested in the recognition of environmental contaminant sources, time-series environmental data analysis, and contaminants’ data and transport analysis and modeling. I have extensive experience with GC/HPLC analysis. My specialty is numerical analysis and model simulation. I have proposed a new idea in source apportionment analysis. I have assisted in teaching several courses on water chemistry and computer-based statistical analysis. I am looking for a research or teaching position at accredited universities or institutes.

Abstract Title: *New idea in source apportionment analysis: A combination of…*

ENVR, GEOC Divisions
30. **Swapnil Liladhar Fegade**, Department of Chemical Engineering, University of North Dakota, 3904 University Avenue, Apt # 3, Grand Forks, ND 58203.

swapnil.fegade@my.und.edu, swapnil.und@gmail.com; C: 701-215-0371, H: 701-777-9083;
University of Mumbai, Institute of Chemical Technology (formerly UDCT), India (B.Tech.,
2005); University of North Dakota (Ph.D., Chem Eng, anticipated Dec 2012), Dr. Brian
Tande, Catalytic reforming of cracked crop oil to produce aromatic compounds.

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

Abstract Title: *Catalytic processes for the production of biobased chemicals and...*

FUEL, ENVR Divisions

31. **Yosra M. Badiei**, Department of Chemistry, Brookhaven National Laboratory, Upton,
NY 11973-5000. ybadiei@bnl.gov; American University in Cairo (B.S., Magna Cum Laude,
Chem, 2003); Georgetown University (Ph.D., Harold Glassman Awardee for Best
Dissertation in Sciences, 2009); Professor Timothy H. Warren, Copper carbenes and nitrenes:
Capture of elusive intermediates and the development of a copper catalyzed C–H amination
reaction; Posdoctoral Associate at Johns Hopkins University (2009–2011), Professor David
P. Goldberg, Oxygen activation using non-heme iron(II) thiolate complexes as synthetic
models for cysteine dioxygenases; Research Associate at Brookhaven National Laboratory
(2011–present), Dr. Etsuko Fujita, Characterization of water oxidation intermediates using
mononuclear ruthenium(II) catalysts.

I seek a tenure-track position mentoring undergraduate and graduate students’ research and
coursework at an academic institution. My research focuses on understanding the role of
transition-metal complexes in mediating electron transfer processes. Highly experienced in
designing, synthesizing, and using a variety of spectroscopic, electrochemical, and analytical
methods for understanding fundamental mechanistic catalytic pathways. I’m currently a team
member researching artificial photosynthesis to produce practical, clean solar fuels. I’ve
supervised many students’ coursework related to general and advanced inorganic chemistry
and mentored multiple research projects. I plan to involve students in multidisciplinary,
collaborative research geared toward their personal and career development.

Abstract Title: *Capture of elusive catalytic intermediates in transition-metal...*

INOR Division
32. Stephen C. Chmely, National Bioenergy Center, National Renewable Energy Laboratory, 15013 Denver West Parkway, Golden, CO 80401. Stephen.Chmely@nrel.gov; Volunteer State Community College (A.S., Chem, 2003); Western Kentucky University (B.S., Chem, 2006); Vanderbilt University (Ph.D., Chem, 2010), Dr. Timothy P. Hanusa, Sterically demanding ligands and their effect on the structure and reactivity of main group metal complexes; Postdoctoral Researcher, Vanderbilt University Department of Biochemistry (Aug 2010–Feb 2011), Dr. F. Peter Guengerich, Mechanistic studies of the human cytochrome P450 19A1 (aromatase); Postdoctoral Research Associate, National Renewable Energy Laboratory (Feb 2011–present), Dr. Gregg T. Beckham, Experimental and computational development of catalysts for the deconstruction of biomass.

I intend to initiate a competitive research program dedicated to the discovery of novel catalytic systems capable of upgrading biomass to fuels and chemicals. My training as an organometallic chemist puts me at the intersection of inorganic, organic, and computational chemistry, and I mean to confer their fundamentals to students. I have assisted in numerous chemistry courses and have developed lesson plans for courses in general chemistry and chemical engineering. I was awarded a departmental research fellowship and a teaching fellowship for exemplary evaluation scores. My dream is to teach and conduct research at a doctoral degree–granting institution.

Abstract Title: Experimental and computational methods for the deconstruction and...

INOR, ORGN, COMP Divisions

33. Elizabeth R. Essinger-Hileman, Department of Chemistry, Pennsylvania State University, 104 Chemistry Building, University Park, PA 16802. ere123@psu.edu; University of New Haven (B.S., Chem and Forensic Sci, 2008); Pennsylvania State University (Ph.D., 2013), Dr. Raymond Schaak, Toward improved nanosynthesis purification and complex nanoarchitecture construction using M13 bacteriophage and material-specific peptides.

I seek a position at a primarily undergraduate institution, where I want to share my excitement about chemistry and motivate students to explore chemistry through research and further education. My current focus is inorganic nanomaterials with aspects of biological and analytical chemistry. In future research, my aim is to develop a curriculum that exposes students to applications of chemistry early on. I will use my experience in aqueous, low-temperature nanoparticle synthesis and my focus on the interface of nanotechnology and biology to develop laboratory experiments and lectures that engage and excite students regarding opportunities to address global problems through chemistry.

Abstract Title: Biomimetic techniques and aqueous, room temperature synthesis in...

INOR Division
34. Luis C. Fernandez-Torres, Center for NanoScience and Technology, and Department of Chemistry & Biochemistry, University of Notre Dame, 251 Nieuwland, Notre Dame, IN 46556-5670. lfernan3@nd.edu; Penn State University (B.S., 1996); UPR-Mayagüez (M.S., 1998), University of Houston (Ph.D., 2003), Dr. Scott S. Perry (Chem), Investigation of TiC(100) and VC(100): Correlation between surface chemistry and microscale tribological properties; Postgraduate Researcher at Penn State University (2003–2005), Dr. Paul S. Weiss, STM studies of substrate-mediated interactions; Assistant Professor of Chemistry at UPR-Cayey (2005–2009); Research Assistant Professor at University of Notre Dame (2009–present), Synthesis and exploration of novel chemical routes for semiconductor nanostructures to use in photovoltaics.

My goal is to establish a research program in materials chemistry, catalysis, surface chemistry, energy, and tribology. My teaching interests include the use of podcasts to enhance lectures and the mentoring of graduate and undergraduate students. I will conduct research in the synthesis of semiconductor nanostructures, such as nanoparticles and nanowires, using chemical bath deposition. These nanostructures can be incorporated into bulk-heterojunction architectures for photovoltaic devices. Moreover, these new nanostructures have the potential to act as photocatalysts. Other projects will include synthesis and characterization of anti-sintering metal nanoparticles and novel synthesis and tribological characterization of layered transition metal chalcogenides.

Abstract Title: *Bulk-heterojunction materials for photovoltaics: Synthesis and…*

COLL, PHYS Divisions

35. Thomas G. Gardner, Department of Chemistry, Gustavus Adolphus College, 800 West College Avenue, Saint Peter, MN 56082. tgardner@gustavus.edu; 612-840-4847; Macalester College (B.A., 1984); University of Illinois (Ph.D., 1989), Dr. Gregory S. Girolami (Chem), Synthesis and characterization of early transition metal complexes with the tripodal phosphine ligand t-butyltris(dimethylphosphinomethyl)silane (“trimpsi”); Postdoctoral Researcher at University of Minnesota (1989–1990), Dr. Louis H. Pignolet, Catalytic activity and scanning tunneling microscopy of heterobimetallic gold clusters; Postdoctoral Researcher at University of Iowa (1990–1991), Dr. Richard F. Jordan, Macrocyclic organozirconium complexes as olefin polymerization catalysts.

As an experienced chemical educator at the undergraduate and graduate levels, I am currently entering my second year as a Visiting Assistant Professor at Gustavus Adolphus College, working with research students on the synthesis of functional materials from phthalocyanines, porphyrins, and other polycyclic aromatic heterocycles with peripheral binding capability. I have taught inorganic, organic, and analytical chemistry and developed special-topics courses in the science and writing of science fiction (Science Fiction Science), nuclear technology in society (Life with the Atom), computational chemistry, and materials science. I seek to teach and supervise research at either the undergraduate or graduate level.

Abstract Title: *Functional supramolecular constructs of edge-binding …*

INOR, ORGN Divisions
36. **Zachariah M. Heiden**, Center for Molecular Electrocatalysis, Chemical and Material Sciences Division, Pacific Northwest National Laboratory, P.O. Box 999, K2-57, Richland, WA 99352. Zachariah.Heiden@pnnl.gov; 509-375-2745; University of Wisconsin–Madison (B.S., chem eng and chem, 2004); University of Illinois at Urbana-Champaign (Ph.D., 2008), Prof. Thomas B. Rauchfuss, Small molecule activation using transfer hydrogenation catalysts; Postdoctoral Fellow at the University of Toronto (2008–2011), Prof. Douglas W. Stephan, Development of an asymmetric metal-free hydrogenation catalyst; Postdoctoral Fellow at Pacific Northwest National Laboratory (2011–present), Dr. R. Morris Bullock, Dinitrogen activation with iron-based complexes containing pendant bases.

I am pursuing a professorship at a Ph.D.- or M.S.-granting institution, where I plan to manage an active research group and train and mentor future scientists. In this role, I seek to teach general, inorganic, and physical chemistry at any level. My research interests broadly lie in the areas of main group and transition metal chemistry, focusing on the applications of catalysis, energy, photochemistry, biological modeling, and mechanistic analysis. I hope to interest students in chemistry, biochemistry, and chemical engineering in my research and teaching.

Abstract Title: *Using general chemistry concepts in cutting edge catalytic…*

INOR, CATL, FUEL, PHYS Divisions

37. **Monty Liong**, Center for Systems Biology, Massachusetts General Hospital–Harvard Medical School, 185 Cambridge Street, Boston, MA 02114. liong.monty@gmail.com; University of California, Los Angeles (B.S., 2004; Ph.D., 2009), Prof. Jeffrey I. Zink, Biomedical applications of mesostructured silica materials; Research Fellow at Massachusetts General Hospital (2009–present), Prof. Ralph Weissleder, Multiplexed labeling and signal amplification in diagnostic magnetic resonance.

My research will use materials and bioconjugate chemistry to address current needs relating to personal therapeutics and diagnostics. Specifically, I plan to focus my areas of interest in: 1) engineering cells for immunotherapy, 2) developing noninvasive diagnostics for circulating biomarkers, and 3) using inorganic nanomaterials for both microscopic and macroscopic imaging. My research and teaching experience in a chemistry department and at a research hospital have demonstrated how the multidisciplinary fields of science, engineering, and medicine can advance progress in biomedical research.

Abstract Title: *Inorganic nanomaterials: Functional scaffold in therapeutics and…*

INOR, BIOL, COLL Divisions
38. Tianbiao Liu, Chemical and Material Sciences Division, Pacific Northwest National Laboratory, P.O. Box 999, K2-57, Richland, WA 99352. Tianbiao.Liu@pnnl.gov; Hubei University of Technology, China (B.S., 2000); Dalian University of Technology, China (M.S., 2004), Professor Licheng Sun, Synthesis and electrochemical studies of iron–sulfur clusters; Texas A&M University (Ph.D., 2009), Prof. Darenbourg, Organometallic complexes that model the active sites of the [FeFe] and [mono-Fe] hydrogenases; Postdoctoral Researcher at Pacific Northwest National Laboratory (2009–present), Dr. Daniel DuBois and Dr. Morris Bullock, Half-sandwich Fe/Ru complexes containing built-in proton relays as efficient electrocatalysts for catalytic H₂ oxidation–production and homogenous catalysts for N₂ reduction.

My research interests spread broadly through inorganic and organometallic synthesis, homogenous and electrochemical catalysis, and bioinorganic chemistry to address challenges of renewable energy, environmentally benign chemical transformations, and redox-active metal complexes of biological or medicinal importance. I have two years of teaching experience in general chemistry and organic chemistry and four years of research mentoring experience with undergraduate and graduate students. I am pursuing professorship at a Ph.D.-granting institution where I will manage an active research program involving undergraduate students and graduate students. I can teach courses in my area of expertise for both undergraduate and graduate students.

Abstract Title: *Half-sandwich Fe electrocatalysts for H₂ oxidation and production*

INOR Division
39. Heather R. Lucas, National Institute on Aging, National Institutes of Health, 251 Bayview Boulevard, Room 05B129, Baltimore, MD 21224. lucash@mail.nih.gov; Randolph-Macon College (B.S., 2002), Dr. Serge Schreiner (Organometallic), Synthesis and characterization of new iridium diphosphine complexes; Johns Hopkins University (M.A., 2005; Ph.D., 2008), Dr. Kenneth D. Karlin (Synthetic Bioinorg) and Dr. Gerald J. Meyer (Physical Inorg/Photochem), Ligand influences on the photoinitiated binding of small molecules to synthetic copper and heme-copper complex systems; Visiting Fellow at Osaka University (2008), Dr. Shunichi Fukuzumi (Electron Transfer Chem), Mononuclear copper complex catalyzed four-electron reduction of oxygen; Lenfant Biomedical Fellow at National Heart, Lung, and Blood Institute (2008–2011), Dr. Jennifer C. Lee (Molecular Biophysics), Copper(II/I) binding to soluble, fibrillar, and/or membrane-bound α-synuclein; Postdoctoral Fellow at National Institute on Aging (2011–2012), Dr. Joseph M. Rifkind (Biochem/Hematology), Effect of copper associated amyloid-β on red blood cell physiology and inhibition by polyphenols.

My goal is to obtain a tenure-track faculty position at a Ph.D.-granting institution where I can establish a well-funded research program and successfully educate a diverse student population. The multidisciplinary nature of my research will provide opportunities for individuals at all levels who are interested in inorganic or biological chemistry, or both, as well as photochemical techniques. My approach will involve (i) examining metal–protein interactions and subsequent reactivity, (ii) characterizing synthetic model systems to elucidate general coordination properties and reactivity patterns, (iii) small molecule photodissociation from variable metallocenter complexes, and (iv) investigating putative metalloprotein active sites through peptide analogs.

Abstract Title: *Amyloids and copper biochemistry: Effects of metal dyshomeostasis in…*

INOR, BIOL, PHYS Divisions

40. Molly A. O'Connor, Department of Chemistry, Drexel University, 3141 Chestnut Street, Philadelphia, PA 19104. maoconnor83@gmail.com; 717-891-7897; Albright College (B.S., 2005); Drexel University (Ph.D., anticipated Aug 2012), Dr. Anthony W. Addison, Chiral and achiral Cu(II) and Ni(II) complexes with novel multidentate ligands.

I am seeking a faculty position at a primarily undergraduate institution. As a faculty member, I hope to instill an appreciation for chemistry in students through course instruction and undergraduate research. I have teaching experience in a wide range of lecture and laboratory courses, including general chemistry, organic chemistry, and inorganic chemistry. My research interests lie in the preparation and characterization of chiral small molecule metal complexes.

Abstract Title: *Chiral and achiral Cu(II) and Ni(II) complexes with novel…*

INOR Division
41. Matthew S. Remy, Department of Chemistry, the Pennsylvania State University, 104 Chemistry Building, University Park, PA 16802. mrs32@psu.edu; Grand Valley State University (B.S., 2005); University of Michigan (Ph.D., 2011), Prof. Melanie S. Sanford, Group 10 methyl transfer reactions toward catalyst development for oxidative oligomerization of methane; Postdoctoral Scholar at the Pennsylvania State University (2011–present), Prof. Raymond E. Schaak, Hybrid nanoparticles in organic and organometallic chemistry.

My teaching background includes: assistant for general and organic chemistry classes, substitute lecturer for a 400-level inorganic class, and developing a training curriculum for graduate student instructors. In addition to lecturing, my goal is to interest students in organometallic, materials, and computational chemistries through the design of molecular models of surfaces of catalytic materials. These compounds will be tested for catalytic activity and ability to activate small molecules such as CH4, O2, N2, CO2, etc. NMR, IR, and gas chromatography will be the major analytical techniques, and kinetics and quantum chemical calculations will be commonly used tools.

Abstract Title: **Catalyst development on the molecular and nano scales**

INOR Division

42. Andrew J. Roering, Department of Chemistry and Biochemistry, University of San Diego, 5998 Alcala Park, San Diego, CA 92110. aroering@sandiego.edu; St. Cloud State University (B.S., Chem, 2006), The University of Vermont (Ph.D., 2011), Dr. Rory Waterman, P–C and P=C Bond formation of a zirconium complex via stoichiometric and catalytic insertion reactions; Postdoctoral Research Associate at University of San Diego (2011–present), Dr. Timothy B. Clark, Substrate directed C–H borylation reactions of benzylic amines; Copper catalyzed diborations of aldehydes and ketones.

I am interested in establishing my own research group in the field of synthetic inorganic chemistry with a focus on catalysis. My research will involve the synthesis of new metal complexes for their use in catalytic bond-forming reactions. I have training in synthetic organometallic chemistry, as well as in teaching organic chemistry. My current position as a postdoctoral researcher at an undergraduate institution has given me the opportunity to mentor several undergraduate research students. It is in this research environment at a primarily undergraduate institution that I would like to launch my career as an independent researcher.

Abstract Title: **Synthesis and reactivity of transition-metal catalysts for main group…**

INOR, ORGN Divisions
43. **R. Bryan Sears**, Wellman Center for Photomedicine, Massachusetts General Hospital, Harvard Medical School, 40 Blossom Street, Boston, MA 02114. Sears.Bryan@mgh.harvard.edu; 614-551-2928; Georgia Southern University (B.S., 2005); The Ohio State University (M.S., 2007; Ph.D., 2010), Dr. Claudia Turro, Photochemical and spectroscopic studies of ruthenium(II) complexes as potential photodynamic therapy agents; Postdoctoral Researcher at Harvard Medical School (2011–present), Dr. Tayyaba Hasan, Using nanotechnology for multi-compartmentalized delivery of photosensitizer and c-Met inhibitor to enhance treatment of cancer.

I have a passion for science and a desire to share that enthusiasm with students. In the past seven years, I have served as a general chemistry instructor and undergraduate research mentor. My experience has taught me the satisfaction that comes from illuminating the tangible chemistry that occurs every day for everyone. My research interests focus on using photoactivated inorganic complexes as potential chemotherapies and aim to promote student involvement in this pursuit. I see myself functioning at peak performance within a liberal arts school setting. In particular, I am interested in colleges with a strong commitment to undergraduate research.

Abstract Title: *Development of novel therapeutics, combinations, and formulations…*

INOR, MEDI Divisions

44. **Laura Strausberg**, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, VA 22904. ljs3t@virginia.edu; Hollins University (B.A., 2008); University of Virginia (Ph.D., anticipated July 2013), Dr. W. Dean Harman, Small molecule functionalization through dearomatization.

My experience teaching laboratory courses to general chemistry and honors students and mentoring undergraduate research students has impressed upon me the importance of hands-on experience in chemical education. I would like to develop courses that emphasize learning-by-doing in general, inorganic, and organic chemistry. My research interest is in exploring characteristics and reactivity of metal complexes for synthesizing novel organic molecules. I am interested in teaching at a primarily undergraduate institution that will afford me the opportunity to work closely with students in developing their skills and understanding of synthetic chemistry.

Abstract Title: *Stereoselective modifications of naphthalene: An undergraduate project…*

INOR, ORGN Divisions
45. Emily Garcia Sega, Department of Chemistry, Ithaca College, 953 Danby Road, Ithaca, NY 14850. egarciasega@ithaca.edu; 607-274-7105; Seton Hall University (B.S., 2006); University of California, San Diego (Ph.D., 2011), Professor Thomas Hermann, Targeting RNA with small molecules: Dihydropyrimidinone derivatives as novel RNA-binding ligands; Postdoctoral Teaching Fellow at Ithaca College Department of Chemistry (2011–present), Interrupting bacterial communication: Investigating small molecules for quorum sensing regulation.

I am seeking a teaching and research position at a primarily undergraduate institution. As a postdoctoral teaching fellow, I have had the opportunity to mentor undergraduate students in independent research endeavors as well as in coursework. My research involves the design, synthesis, and biological evaluation of small molecules as potential antibacterial agents. In the classroom I am committed to teaching excellence and have taught both introductory and upper elective courses. I strive to create classroom and laboratory environments of attentive, active learning where students can further develop their ability to think critically.

Abstract Title: Interrupting bacterial communication: The design and synthesis of...

46. Sunny M. Ogbomo, Department of Pharmaceutical Sciences, University of Nebraska Medical Center, Omaha, NE 68198. sunnyogbomo@yahoo.com; 817-745-3503; Ambrose Alli University, Nigeria (B.Sc., 1987); Memorial University of Newfoundland, St. John’s, NF, Canada (M.Sc., 1996); University of North Texas, Denton, (Ph.D., 2009), [Professor and research topic unknown]; Postdoctoral Fellow at University of Nebraska Medical Center (2010–present) [Professor and research topic unknown].

Developing metabolically active conjugates to enhance polymer-based drug delivery systems for diagnostic imaging and radiotherapeutic applications in pancreatic adenocarcinoma patients is at the forefront of my research. My future interests entail developing targeted molecular imaging and radiotherapeutic agents, magnetic nanoparticles, and biodegradable polymers for cancer diagnosis and therapy, polymer micelle based drug delivery, as well as devices and biomaterials and gold nanoparticles relating to biomarkers. I have taught general chemistry and organic chemistry lab courses and I look forward to pursuing my passion for teaching and research at a four-year college or comprehensive university.

Abstract Title: Drug delivery in pancreatic cancer and effort in reducing toxicity

MEDI, ORGN Divisions
47. Nicholas P. Bizier, Department of Chemistry, Colby College, 5750 Mayflower Hill, Waterville, ME 04901-8857. npbizier@colby.edu; Colby College (B.A., 2001); Montana State University (Ph. D, Org Chem, 2008), Dr. Mary Cloniniger, The use of In(OTf)3 as a Lewis Acid in carbohydrate chemistry, and exploration in silicon tethered reactions; Research Scientist at John I Haas (2008–2011); Postdoctoral Fellow at Colby College (2011–present), Dr. Jeffery Katz, Synthesis of diazadioxacaliz[4]arenes, and Electron withdrawing capabilities of alkynes.

I am seeking a tenure-track position at an undergraduate-only institution, where my primary focus will be teaching undergraduate courses and leading undergraduates in research activities. I have experience in teaching at the classroom and the laboratory level. As a graduate student and as a postdoctoral fellow I mentored undergraduates. I also bring to the classroom the unusual experience of having practiced chemistry in an industrial setting for two years. My research interests include developing novel synthetic pathways to biologically active compounds.

Abstract Title: Single step, regioselective synthesis of diazadioxacalix[4]arenes and…

ORGN Division

48. Richard T. Desmond, Department of Chemistry, University of Connecticut, 55 North Eagleville Road Unit 3060, Storrs CT 06269. Richard.desmond@uconn.edu; 860-486-6467; College of The Holy Cross (B.A., Chem, 2001); NSF EAPSI Summer Fellow at Nanyang Technological University, Singapore (2010), Dr. Brendan P. Orner, (NSF-funded project investigating cyclic peptide libraries for organocatalytic activity) Synthesis of cyclic peptide library using split-intein circular ligation of peptides and proteins; Expression of maltose-binding protein; University of Connecticut (Ph.D., Chem, anticipated fall 2012), Dr. Mark W. Peczuh, Synthesis and biological evaluation of natural-product–like macrolactones fused to carbohydrates.

I want to share my enthusiasm for basic research and appreciation for small institutions while teaching at a small PUI. I’ve TA’d general and organic chemistry programs and mentored three undergraduates’ independent research for the NSF’s REU Program. All pursued graduate school and two authored manuscripts together. As a supervisory TA in general chemistry at PSU, I trained TAs, managed their administrative duties for multiple section courses, and developed lab curricula. PSU recognized me with a teaching award in 2004; UConn followed suit in 2008. Teaching undergraduates and a passion for chemistry are the principal reasons I pursued a Ph.D.

Abstract Title: Synthesis and biological evaluation of natural product-like macrocycles…

ORGN, CARB, MEDI, BIOL Divisions
49. Ethan L. Fisher, Department of Chemistry, University of California, Berkeley, Berkeley, CA, 94720. ethanf@berkeley.edu; University of Pennsylvania (B.A., 2006); Columbia University (M.A., 2007; M.Phil., 2010; Ph.D., 2011); Prof. Tristan Lambert, Progress toward the total synthesis of platensimycin and study of aromatic ions: Carbon-based nucleofuges and chiral cyclopropenones and formamides; Postdoctoral Scholar at the University of California, Berkeley (2011–present), Prof. Richmond Sarpong, Total synthesis of diterpenoid alkaloids and metal catalyzed cycloisomerizations.

I am seeking a faculty position at a four-year college focused on undergraduate teaching and research. The subdiscipline of organic chemistry especially interests me. My research interests include developing small molecules containing both Lewis acidic and Lewis basic sites for use in catalysis and also the engineering of geometrically controlled reagents for site-selective reactivity. My teaching experience spans more than five years of both organic chemistry lecture and laboratory sections, recognized in 2010 with a teaching award in graduate school. With my past and current experience in teaching and research, I intend to develop a strong curriculum for undergraduate students.

Abstract Title: **Tungsten catalyzed heterocycloisomerizations and the total synthesis…**

ORGN Division

50. Juliet Hahn, Department of Chemistry, New Mexico Tech, Socorro, NM 87801. JulietHahnPHD@yahoo.com, http://JulietHahn.com; 575-495-1159; University of South Carolina–Columbia (B.S., Magna Cum Laude, Phi Beta Kappa, Chem, [Year unknown]); State University of New York–Stony Brook (Ph.D., Orgn Chem, [Year unknown]), Prof. William leNoble, Stereoselectivity in heterocyclic amine; Postdoctoral Researcher at Columbia University ([Years unknown]), Prof. Gerard Parkin, Transition metal organometallic pyrazoylborates, Cp metallocenes, and salen complexes of interest as metalloenzyme models and polymerization catalysts; Postdoctoral Researcher at University of Wisconsin–Madison ([Years unknown]), Prof. Richard Hsung, Synthetic organic chemistry—heterocyclic amine and pyrone synthesis, enamides and nonnatural amino acid chiral auxiliary of natural products of potential pharmaceutical interest.

Experienced, excellent educator and PI researcher: documentation of excellent college-level teaching (see teaching evaluations on website) and increasing enrollment. Teaching: Organic, General Chemistry lecture and lab, Organometallics, Bioorganic, Organic Spectroscopy, Advanced Organic (class size, 15–300, 95% white, 85% African American, 30% Hispanic, economically disadvantaged, honors students. Research as Principal Investigator with undergraduates: (a) Carbon nanotube materials—solar energy, (b) Photodimerization of DNA base—Experimentally bioorganically model skin cancer, (c) Stereoselective synthetic methodology—Potential pharmaceuticals for Alzheimer’s, and (d) Teaching large lectures and quickly conducting research with undergraduates. Preferred institution: Primarily undergraduate college.

Abstract Title: **How to teach anything to anyone while increasing enrollment and…**

ORGN, BIOL, INOR, Divisions
51. Dahlia Haynes, Department of Chemistry, Carnegie Mellon University, 4400 Fifth Avenue, Mellon Institute Room 846, Pittsburgh, PA 15213. dahliah@andrew.cmu.edu; 412-268-5101; Claflin University (B.S., Chem, 2003); Clemson University (Ph.D., 2008), Dr. Dennis W. Smith, Jr., Novel lactide-derived polymers: Synthesis, properties, and applications; Postdoctoral Research Associate at Carnegie Mellon University (2009–present), Dr. Richard D. McCullough, Conjugated polymer synthesis and self-assembly processes in OFETS and photovoltaics for organic electronic applications.

My current research interest involves the design and synthesis of conjugated block copolymers toward structure–property relationships with distinct focus on the influence on self-assembly and electronic properties, particularly of organic electronic applications. The idea is to control self-assembly in nanostructured materials that can strongly affect the internal processes associated with energy transfer and conversion in polymeric devices. I am pursuing an academic position at an R1 institution where my objectives as a full professor will enable me to demonstrate my commitment to increasing diversity in higher education, while also instilling in my students the importance of contributing to scientific research.

Abstract Title: *Influence of varied polymer and end group moieties on the…*

POLY, PMSE, ORGN Divisions

52. Tanay Kesharwani, Bard College, P.O. Box 5000, Annandale-on-Hudson, NY 12504. tkesharw@bard.edu; Indian Institute of Technology, Mumbai, India (B.S./M.S. (Integrated), Chem, 2002), Dr. Sambasiva R. Kotha, Development of new synthetic methodologies; Iowa State University (Ph.D., Chem, 2008), Dr. Richard C. Larock, Studies in electrophilic cyclization, palladium migration, and cationic polymerization; Postdoctoral Fellow in the Department of Drug Development, NewLink Genetics, Ames, Iowa (2008–2010), Traditional and combinatorial approaches for the synthesis and SAR studies of IDO inhibitors; Postdoctoral Fellow at Northwestern University (2010–2011), Dr. SonBinh T. Nguyen and Dr. Joseph T. Hupp, Design and synthesis of porous organic polymers (POPs) and metal organic frameworks (MOFs) and the study of their applications for gas storage and catalysis.

My research interests focus on developing new synthetic methods and applying them toward the synthesis of novel materials and small molecules of biological interest. Some of my current research interests include developing new efficient chemical transformations using late-transition-metal catalysts, developing green methods in organic synthesis, and designing and synthesizing porous organic polymers (POPs) and metal organic frameworks (MOFs) and their applications in hydrogen storage and catalysis.

Abstract Title: *Electrophilic cyclization: Application in synthesis of biologically…*

ORGN Division
53. **Ajay Mallia**, Department of Chemistry, Georgetown University, Washington DC 20057. amm272@georgetown.edu; University of Kerala, India (Ph.D., 2002), Prof. S. Das, Photochemical phase transitions in supramolecular liquid crystals; JSPS Fellow at National Institute of Advanced Industrial Science and Technology, Japan (2002–2005), Prof. N. Tamaoki, Photoactive liquid crystals for displays and erasable full-color recording; Postdoctoral Fellow at City University of New York (2005–2006), Prof. G. John, Preparation, assembly, and characterization of metal nanoparticles using liquid crystals as templates; Postdoctoral Fellow at Georgetown University (2006–present), Prof. Richard Weiss, Characterization of nanomaterials such as molecular gels and liquid crystals; Adjunct Professor at University of Maryland, College Park and University of the District of Columbia (2011–present).

I am pursuing professorship at a Ph.D.-granting institution or four-year undergraduate college. My research background is in the area of organic nano-architectures. Through my research over the years I became an expert in and developed an appreciation for both theoretical and practical aspects of nanotechnology. My diverse research interests have been featured in 29 peer-reviewed publications. (One of my recent publications appeared as cover feature in J. Am. Chem. Soc. (for details, see http://www.amallia.org/publications.html). I am also actively involved in college-level teaching at the University of Maryland and the University of the District of Columbia as an Adjunct Professor.

Abstract Title: **Self-assembly and fibrillar structures of molecular gels derived from…**

ORGN, ENVR, PHYS, COLL Divisions

54. **Jeremy R. Niskala**, Materials Sciences Division, Lawrence Berkeley National Laboratory, 1 Cyclotron Road – 21 Lewis Hall, Berkeley, CA, 94720. jeremyniskala@gmail.com; 919-260-9914; University of Wisconsin–Superior (B.S., 2006); University of North Carolina at Chapel Hill (Ph.D., Chem, 2010), Dr. Wei You, Design, fabrication, and characterization of molecular junctions; Postdoctoral Fellow at Lawrence Berkeley National Laboratory (2011–present), Dr. Jean M. J. Frechet, Study of new materials for high-performance organic photovoltaics and field effect transistors.

I am interested in organic and inorganic–organic hybrid materials and their application as cheap, flexible, and solution-processible electronics. Particular areas of interest include: fundamental charge transport mechanisms, spin-polarized electron transport in organic materials, new inorganic–organic device architectures, loss mechanisms and defect formation in organic electronics, and the synthesis of new, high-performance organic materials. I hope to obtain a tenure-track position at a research-oriented university that will allow me to both teach and conduct original research. I plan to establish a research lab that is complementary to existing work in the department and competitive within the organic electronics community.

Abstract Title: **From single molecule to device: Building a better understanding of…**

INOR, ORGN, PMSE, POLY Divisions
55. Aditi Patil, Department of Chemistry, University of Illinois at Chicago, 845 West Taylor Street, 4500 SES, Chicago, IL 60607. aditip.111@gmail.com; University of Pune, India (B.S, 2004; M.S., 2006); University of Illinois at Chicago (Ph.D., anticipated Dec 2012), Dr Laura L. Anderson, Study of the coupling reactions of oximes with boronic acids and their subsequent sigmatropic rearrangements.

My research interests are in using organic and organometallic chemistry to develop new methodologies that could be used to overcome current challenges in organic synthesis. I am also interested in devising novel catalytic systems for asymmetric halogenation and amination reactions. For five years, I have had excellent opportunities to hone my teaching skills through a variety of general and organic chemistry classes, including laboratory courses and chemistry for health professionals. I seek to teach and mentor students in a primarily undergraduate institution.

Abstract Title: Synthesis of alpha-hydroxy ketones and aldehydes via the dioxygenation...

ORGN Division

56. Aaron Van Dyke, Department of Chemistry, University of Michigan, 930 N. University Avenue, Room 2716, Ann Arbor, MI 48106. vandya@umich.edu; 734-615-8565; Seattle University (B.S., Chem, 2004); Massachusetts Institute of Technology (Ph.D., Orgn Chem, 2009), Prof. Timothy F. Jamison; Synthetically versatile templates for epoxide-opening cascades; American Cancer Society–Michigan Cancer Research Fund Postdoctoral Fellow, University of Michigan (2009–present), Prof. Anna K. Mapp, Design and synthesis of small molecule transcriptional modulators.

As the product of a liberal arts education, I seek a career at a PUI with a lively research culture. My research interests combine my training as a synthetic organic chemist and chemical biologist, using small molecules to control and study biological systems. Undergraduates in my group will gain experience not only in classical subdisciplines (organic/biochemistry) but also the evolving chemical biology interface. As a teacher–scholar, I have designed research projects tailored to both undergraduate and graduate students and mentored them in the lab. Additionally, I have co-instructed an advanced organic chemistry elective for undergraduates at the University of Michigan.

Abstract Title: Controlling recruitment of transcriptional complexes with bifunctional...

ORGN, BIOL, MEDI Divisions
My research interests focus on gaining a comprehensive understanding of the dynamical behavior of molecular systems and how this knowledge can be applied to a variety of systems, including new solar materials and biopolymers. I wish to conduct multidisciplinary research through collaborations with experimentalists that cross traditional scientific boundaries, and to motivate scientific inquiry in undergraduate and graduate students alike. I have taught general and physical chemistry laboratories and have assisted with undergraduate physical chemistry and graduate statistical mechanics courses. I would like to teach and establish a research program at a college or university that grants advanced degrees.

Abstract Title: Better living through quantum chemistry

PHYS, COMP Divisions

I am interested in developing simulation algorithms to better understand aggregation processes, including atmospheric aerosol formation and the assembly of complex nanostructures in the liquid phase. I have previously taught undergraduate general chemistry laboratories and recitations and physical chemistry laboratory. I plan to take advantage of the unique ability of simulation to provide detailed molecular-level insight not only in the laboratory, but also in the classroom, where movies, snapshots, and simple computer experiments can help students visualize difficult concepts. I would like to teach and supervise the research of undergraduate and possibly master’s degree students at a four-year university.

Abstract Title: Predictive molecular simulations of nucleation phenomena and phase…

COMP, PHYS Divisions
59. **Heather J. Kulik**, Department of Chemistry, Stanford University, Mailbox #136, Mudd Building, Room 121, 333 Campus Drive, Stanford, CA 94305. hkulik@stanford.edu; The Cooper Union (B.E., 2004); Massachusetts Institute of Technology (Ph.D., 2009); Professor Nicola Marzari (Materials Sci), First principles transition metal catalysis; Postdoc at Stanford University (2010–present), Dr. Todd Martinez, Quantum chemistry on GPUs for large-scale studies of protein structure and enzyme catalysis.

Accurate and efficient electronic structure methods permit the predictive computational study and design of metalloenzymes, molecular catalysts, and catalytic surfaces. I hope to develop this further in a research program at a Ph.D.-granting institution and would involve students in the chemical and biochemical sciences and engineering disciplines. I’ve developed a series of online tutorials teaching the fundamentals of this research. They are read by an international audience and would provide a starting point for hands-on learning tools in my courses. The highly portable, visual nature of my computational research makes it an excellent teaching tool for students of all ages.

Abstract Title: *Predictive and fast: New tools for first-principles catalyst and enzyme...*

PHYS, COMP, BIOL, INOR Divisions

60. **Chris B. Milojевич**, Department of Chemistry, University of Tennessee, 1207 Harmony Lane, Knoxville, TN 37912. cbennett@ion.chem.utk.edu; 540-319-1800; Wofford College (B.S., Chem, 2003); Wake Forest University (M.A., Education, 2004); University of Tennessee (Ph.D., Chem, anticipated May 2013), Dr. Jon Camden, Surface enhanced hyper Raman spectroscopy.

I am interested in spectroscopic techniques and their application to solving various problems. Due to my background as a teacher, I am interested in working at an institute that stresses teaching, but would also like to lead an undergrad research group. I have spent much of my graduate career staying involved in community outreach, curriculum development, leadership, and mentoring, and I am looking for a position where those skills can be put to use.

Abstract Title: *Nonlinear laser spectroscopy used as a molecular probe*

ANYL, PHYS Divisions
61. **David Alexander Sivak**, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Mailstop: Stanley, Berkeley, CA 94720. dasivak@lbl.gov; Harvard College (A.B., 2000); University of California, Berkeley (Ph.D., Biophysics, 2009), Prof. Phillip L Geissler (Chem), DNA bending elasticity; Physicist Postdoctoral Fellow at Lawrence Berkeley National Laboratory (2009–present), Dr. Gavin E. Crooks (Physical Biosci), Nonequilibrium statistical mechanics.

I seek a tenure-track faculty position at a research university. My primary research is directed toward using theoretical and computational techniques, in close collaboration with experimentalists, to study the non-equilibrium thermodynamics of molecular-scale biological processes. My future research plans seek to understand the non-equilibrium efficiency of molecular machines, their ability to convert input energy into useful work. My ultimate aim is to discover the basic principles of driven molecular-scale energy conversion, in order to explain biomolecular machines’ complex evolutionary optimization and to provide design principles for synthesizing artificial molecular machines toward such ends as drug delivery or photosynthesis.

Abstract Title: *Nonequilibrium thermodynamics of biomolecular machines*

PHYS, COMP Divisions

62. **Adam H. Steeves**, Department of Pharmaceutical Chemistry, University of California, San Francisco, 600 16th Street, San Francisco, CA 94158. Adam.Steeves@ucsf.edu; Williams College (B.A., 2002); Massachusetts Institute of Technology (Ph.D., 2009), Robert W. Field, Electronic signatures of large amplitude motions; NIH Postdoctoral Fellow at UCSF (2010–present), Dr. Matt Jacobson, Dr. John Gross, and Dr. David Morgan, Conservation of allosteric mechanisms within an enzyme family.

I am seeking a faculty position in physical chemistry at a primarily undergraduate institution. My research interests involve applying fundamental physical chemistry approaches to understanding the regulatory mechanisms of biomolecules. I address this problem using spectroscopic and computational techniques to probe interactions between proteins and small molecules, and the conformational changes that such an interaction can produce. I look forward to mentoring undergraduates in an interdisciplinary and collaborative research environment.

Abstract Title: *Spectroscopic and computational approaches to understanding enzyme...*

PHYS Division
63. Luis Velarde, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, 902 Battelle Boulevard, P.O. Box 999, MSIN K8-91, Richland, WA 99354. luis.velarde@pnnl.gov; Monterrey Institute of Technology and Higher Education (B.S., 1998); New Mexico Tech (M.S., 2001), Dr. Larry Werbelow, NMR lineshapes of molecular relaxation processes in spin-coupled systems; University of Arizona (Ph.D., 2008), Dr. Andrei Sanov, Electronic structure and photo-initiated dynamics of mass-selected anions (experiment); President’s Postdoctoral Fellow at University of California, Santa Barbara (2008–2010), Dr. Alec Wodtke, Molecule-surface scattering with highly vibrationally excited molecular beams; Postdoctoral Research Associate at Pacific Northwest National Laboratory (2010–present), Dr. Hong-fei Wang, High-resolution nonlinear laser spectroscopy and ultrafast dynamics at surfaces and interfaces.

My overall scientific interest pivots on molecular-level understanding of ultrafast surface processes and interfacial molecular organization. I plan to develop a vigorous research program using and developing novel nonlinear laser spectroscopy methods and cutting-edge surface science techniques for detailed investigation of emergent phenomena at oxide and charged interfaces. Most of all, I wish to provide an environment for students to cultivate career and life skills, a creative problem-solving mindset, and the capacity for scientifically driven critical thinking. I therefore seek a faculty position at a research university, where I look forward to teaching and mentoring graduate and undergraduate students.

Abstract Title: Surface-specific vibrational line shapes with sub-wavenumber resolution:…

PHYS, COLL, ANYL, COMP Divisions

64. Nicholas D. Ball, Department of Chemical Engineering, California Institute of Technology, 1200 E. California Boulevard, MC 210-41, Pasadena, CA 91125. nball@caltech.edu; 626-395-2510; Macalester College, (B.A., Chem, 2005); University of Michigan, (NIH Predoctoral Research Fellow, Ph.D., Chem, 2010), Prof. Melanie S. Sanford, Synthesis and study of high-oxidation Pd compounds towards the development of catalytic C–F and C–CF3 bond-forming reactions; NIH Postdoctoral Fellow at California Institute of Technology (2011–present), Prof. David A. Tirrell, Development of selenium-based biomaterials responsive to reactive oxygen species (ROS).

I would like to introduce a research program focused on designing and synthesizing metal catalysts with applications in renewable and environmental chemistry. Catalytic methods will be developed to (1) introduce small greenhouse gases into organic molecules, and (2) convert biomaterials and synthetic polymers into chemical feedstocks. With my experience as a mentor of both undergraduate and graduate students, my goal is to provide an opportunity to translate theory into experiment and develop valuable problem-solving skills. I am interested in teaching and mentoring students in synthetic organic and inorganic chemistry and material science at a research-oriented four-year college or university.

Abstract Title: Selenoamino acids and the development of biomaterials responsive to…

ORGN, INOR, POLY Divisions
65. Arun K. Kota, Department of Materials Science and Engineering, University of Michigan, 2216 HH Dow Building, 2300 Hayward Street, Ann Arbor, MI 48105. arunkota@umich.edu; Andhra University (B.Tech., Chem Eng, 2001); Clarkson University (M.S., Chem Eng, 2003); University of Maryland (Ph.D., Mech Eng, 2008); Dr. Hugh A. Bruck, Processing–structure–property relationships of polymer–carbon nanotube/nanofiber composites; Postdoctoral Researcher at University of Pennsylvania (2008–2009), Karen I. Winey, Micellar morphology in sulfonated pentablock copolymer solutions; Postdoctoral Researcher at University of Michigan (2009–present), Anish Tuteja, Superhydrophilic and superoleophobic surfaces for effective oil–water separation, hierarchically structured superoleophobic surfaces, electric-field driven actuation of liquids.

I intend to pursue an academic career at a doctorate-granting university because I enjoy both research and teaching in equal measure. I plan to build a research program aimed at understanding and engineering functional nanoparticle–polymeric systems. The specific surface and bulk properties of the materials developed through this work will address some of the key challenges in the areas of environmental science and energy conservation. I can assume the responsibility of teaching most undergraduate or basic graduate courses in chemical engineering and materials. I can also teach advanced graduate courses in my area of research expertise.

Abstract Title: Hygro-responsive membranes for effective oil-water separation

PMSE Division
66. Sreekar Babu Marpu, Department of Chemistry, University of North Texas, West Mulberry, Denton, Texas, TX 76203. sreekarmarpu@gmail.com; Osmania University, Hyderabad, India (B.Sc., 1999; M.Sc., 2001); SRM College, Hyderabad, India (Lecturer in Chemistry, 2002–2004); University of North Texas (Ph.D., 2011), Prof. Zhibing Hu and Prof. Mohammad A. Omary, Biocompatible hybrid nanomaterials involving polymers and hydrogels interfaced with phosphorescent molecules and toxin-free metallic nanoparticles for biomedical applications; Postdoctoral Research Associate at University of North Texas, Department of Chemistry (2011–present), Prof. Mohammad A. Omary, Syntheses of multifunctional opto-electronic micro- and nanomaterials for biomedical and energy applications.

I am seeking a faculty position at a research-oriented comprehensive university that will allow me to pursue teaching and research. My research interest is in developing multifunctional nanomaterials for establishing new synthesis techniques and understanding their physiochemical properties for biomedical and energy applications. I thoroughly enjoy teaching and have experience as an instructor and a teaching assistant. I’ve supervised seven students in my current position and am Co-PI on three U.S. pending patents and one university grant proposal. This would provide a unique platform to mentor students in a multidisciplinary, collaborative atmosphere, guiding them into careers in academia or industry.

Abstract Title: *Syntheses and understanding of multifunctional hybrid nanoparticles*

INOR, PMSE Divisions
67. Virendra Singh, The George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, 771 Ferst Drive, Atlanta, GA 30332. vsingh@gatech.edu; 859-221-6444; Indian Institute of Technology, Roorkee (IIITR), India (MS., 2000; M.Phil., 2001); Panjab University (Ph.D., 2007), Prof. Alok Srivastava, Physico-chemical studies of swift heavy ion modified polymers; Postdoctoral Fellow at School of Chemical and Biomolecular Engineering, Georgia institute of Technology, (2007–2009), Prof. Sven H. Behrens, Adsorption and interaction of charged (polymer) colloid particles at oil–water interface and surfactant mediated charging of nonpolar solvents; Postdoctoral Research Associate at School of Mechanical Engineering, Georgia Institute of Technology, (2010–present), Prof. Baratunde A. Cola, Fabrication and characterization of conjugated polymer and CNT-based hybrid nanostructures for improved heat transfer at interfaces.

I intend to establish a research program based on the design and development of hybrid soft materials (polymer and colloid). I am interested in developing polymer hybrid nanomaterials via controlling the constituents’ macroscopic and nanoscale arrangements for enhanced charge transfer at interfaces. I am passionate about teaching and would be interested in teaching Physical Chemistry, Instrumentation, Macromolecules, Colloid/Interface Chemistry, Nanoscience and Nanotechnology (Nanomaterial Fabrication and Applications), and Electrochemistry at the graduate level. I would also be interested in teaching Analytical, General, and Inorganic Chemistry and Polymer Science at the undergraduate level.

Abstract Title: *Macromolecular nanoengineering: Fabrication and characterization*…

PMSE, ANYL, BIOL Divisions
68. **Yashveer Singh**, Department of Pharmaceutics, Ernest Mario School of Pharmacy, Rutgers University, 160 Frelinghuysen Road, Piscataway, NJ 08854.
yashveer_singh_a@yahoo.com; 732-781-6066; University of Purvanchal (B.S., Chem, 1993); University of Gorakhpur (M.S., Orgn Chem, 1996); University of Allahabad (Ph.D., Orgn Chem, 2001), Prof. Krishna Misra, Studies in oligonucleotides of therapeutic value; Postdoctoral Fellow at the Indian Institute of Science (2001–2003), Prof. Santanu Bhattacharya, Membrane sensitive fluorescence probes; Joseph Fourier University (2003–2005), Prof. Eric Defrancq, Oligonucleotide conjugates; Assistant Research Professor, Rutgers University (2005–present), Prof. Patrick J. Sinko, Polymeric drug delivery systems.

I seek a faculty position at a four-year college, a university, or a pharmacy school. Research accomplishments: polymeric biomaterials (nanocarriers, gels, hydrogels) for drug delivery (breast cancer drug and vaginal microbicide). Undergraduate and graduate teaching experience in biochemistry, organic chemistry, pharmaceutical biotechnology, and pharmaceutical sciences. Interests: developing noninvasive optical imaging to detect and monitor disease with high precision and accuracy and measure drug distributions (targeting) in vivo. My research program will actively involve undergraduates. I will teach organic/medicinal chemistry, biochemistry, biotechnology, and pharmaceutical sciences and develop courses in polymer therapeutics, biotherapeutics, and polymeric biomaterials for drug delivery and tissue engineering.

Abstract Title: *Noninvasive optical imaging to investigate the passive distribution of…*

PMSE, POLY, ORGN Divisions

69. **Fernando Uribe-Romo**, No biographical sketch provided

Abstract Title: *Bottom-up synthesis of graphene nanoribbons from poly…*
70. Jasmina C. Cheung-Lau, Department of Chemistry, University of Pennsylvania, 231 S. 34th Street #312; Philadelphia, PA 19104. jasminac@sas.upenn.edu; Amherst College (B.A., Cum Laude, Chem, Music, 2003); University of Pennsylvania (Ph.D., anticipated Aug 2012), Prof. Dmochowski, Interaction of ferritin with nanoparticles and with other small molecules.

My research interests lie in electron-transfer processes—especially within proteins—and the biophysical properties of the proteins in these different states. This research can provide insight toward developing advanced energy storage units. In my research experiences, I have mentored and trained younger undergraduates and graduate students. Furthermore, in graduate school, I taught in college-level courses for more than 10 semesters, varying from laboratory-based to instructional teaching. I am constantly invigorated by the students I encounter and the challenging questions they ask of me. I hope to teach and direct research for undergraduate students at a four-year college.

Abstract Title: **Self-assembly of ferritin around gold nanoparticles**

POLY, COLL Divisions

71. Kimberly A. Milligan, Department of Chemistry, Delaware State University, 1200 North DuPont, Dover, DE 19901. kmilligan@desu.edu; Delaware State University (B.S., 2001; M.S., 2004) Dr. Teresa Singleton (Bio, 2001–2004), Integration events of Tf1, an LTR-retrotransposon, into the host, *Saccharomyces pombe*; Delaware State University (Ph.D., 2012), Dr. Cherese Winstead (Chem, 2008–present), Chitosan nanoparticles for extended release of oxytocin: Applications in autism treatment.

I am interested in using biopolymers as drug delivery systems because of their biocompatible and mucoadhesive properties. I am currently synthesizing chitosan nanoparticles for extended release of oxytocin in order to alleviate some of the symptoms associated with autism. The applications of biopolymers in pharmaceuticals are many, making this area of research very intriguing. I have more than six years of teaching experience in nursing chemistry. I have trained and overseen six undergraduate and two graduate projects in our laboratory. I would like to teach and direct the research of undergraduate students at a four-year college or university.

Abstract Title: **Chitosan nanoparticles for time-released delivery of oxytocin:**

POLY, MEDI Divisions
Research interests center on understanding the mutagenesis potential of DNA-protein cross-links and assessing their value as disease biomarkers. Focus on (1) synthesis of site-specifically modified oligodeoxynucleotides, (2) delineating their repair mechanism, and (3) developing sensitive methodologies to detect these modified DNA lesions in vitro and in vivo. Experimental techniques to be chemical synthesis, chromatography, mass spectrometry, enzyme kinetics, and biomolecule X-ray crystallography. Interests: establishing a research program in an M.S.- or Ph.D.-granting university. Potential courses to teach: (1) undergraduate: general chemistry, instrumental analysis, quantitative analysis, and biochemistry, and (2) graduate: bioanalytical chemistry, chemical toxicology, and nucleic acid chemistry.

Abstract Title: **Mutagenesis: From molecular mechanisms to biomarkers**

TOXI, ANYL, BIOL Divisions
Engineered nanoparticles for biomedical analysis

Elizabeth Crew, ecrew1@binghamton.edu. Department of Chemistry, Binghamton University, State University of New York, Binghamton, NY 13902, United States

Nanoparticles have garnered much interest in recent years for many applications, including green energy, sensing and biomedical applications. From the early years, the simple detection of a target DNA sequence by colorimetric assay to the advanced applications of theranostics, nanoparticles have become a large part of biomedical research. From silver and gold metallic nanoparticles, to polymer and semiconducting quantum dots, each is finding its place in these applications. This presentation will focus on the use of metallic nanoparticles in several applications; focusing on DNA mediated assembly and restriction enzyme disassembly of gold nanoparticles for cancer diagnostics and microRNA modified gold nanoparticles for cell transfection studies. Finally, future directions of this work will be discussed.
Applications of electrochemical techniques to study biological systems: From cancer cells to bacterial biofilms

Dipankar Koley¹,³, dkoley@umich.edu, Lajos Höfler¹, Jianfeng Wu², Chuanwu Xi², Mark E Meyerhoff¹, Matthew M Ramsey⁴, Marvin Whiteley⁴, Allen J Bard³. ¹Department of Chemistry, University of Michigan, Ann Arbor, MI 48109, United States ²School of Public Health, University of Michigan, Ann Arbor, MI 48109, United States ³Department of Chemistry, The University of Texas, Austin, TX 78712, United States ⁴Section of Molecular Genetics and Microbiology, The University of Texas, Austin, TX 78712, United States

A wide variety of electroanalytical techniques, including Scanning Electrochemical Microscopy (SECM), have been used for studying different cell systems. In this presentation, recent developments in the applications of SECM to study cancer cells and microbial biofilms will be reported. Further, efforts to use a novel electrochemical nitric oxide generation method to prevent biofilm formation on polymer surfaces will be described.

With respect to cancer cells, real time quantitative detection of thiodione (menadione-conjugate) pumped out of the HeLa cells by multidrug resistance (MDR) pumps was determined by SECM to be 140 μM when cells are exposed to 500 μM menadione. Selective blocking of these MDR pumps can be achieved (as detected by SECM monitoring of thiodione) by small molecules such as MK571 as well as by the MDR specific antibody. SECM can also be used to study microbial biofilm of P. aeruginosa. Real time detection of pyocyanin produced by a biofilm formed from these bacteria was determined to be 2.5 μM after 6 h. Pyocyanin (PYO) was also observed to be reduced by the biofilm, thus maintaining a reduced PYO atmosphere above the biofilm even in presence of oxygen.

To prevent formation of biofilms on polymers, a novel pulsed electrochemical method to generate and modulate the release of NO, a highly potent and natural bactericidal agent, from inorganic sodium nitrite salt will also be presented. The NO is electrochemically generated by the reduction of nitrite ions by Cu(I) ions generated anodically at the surface of a copper electrode and subsequent cleaning of the rapidly passivated electrode surface by applying a cathodic voltage pulse. This electrochemical approach is adapted to a catheter configuration and shown to dramatically reduce biofilm formation over a period of 7 days with several bacteria. Recent progress in controlling the amount of NO flux released from the catheters as well as a novel planar patch configuration via the use of specific electromodulation voltages and frequency will also be presented.
Small molecule natural products enable microbial growth

*Eric J Dimise*, *Eric_Dimise@hms.harvard.edu*, *Jon Clardy*, *Steven D Bruner*. (1) *Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA 02115, United States*  (2) *Department of Chemistry, University of Florida, Gainesville, FL 32611, United States*

Initiation of microbial growth is dependent upon the state of the environment. Small molecules are typically employed to overcome challenges that would otherwise limit or arrest growth.

Siderophores are small molecules that sequester iron, a growth-limiting essential nutrient. The fuscachelins are peptidic siderophores isolated from *Thermobifida fusca*. We used bioinformatics, assay guided fractionation, NMR and mass spectrometry to determine their structure, which was then confirmed via total chemical synthesis.

Microbes are capable of generating growth-inducing molecules for their neighbors. We have isolated a species from local intertidal sediment and found that it provides quinones and chromenols as growth factors for other species. We are now investigating the unique challenges involved in trafficking lipophilic molecules through an aqueous environment. We also examine the possibility of these ubiquitous compounds as general growth signals and their implication in the cycles of dormancy and active growth in the environment and in the human host.
Natural and nonproteogenic amino acids in natural product biosynthesis

Elisha N Fielding, efielding@ucsd.edu. Center for Marine Biotechnology and Biomedicine, Scripps Institution of Oceanography, UCSD, La Jolla, CA 92037, United States

Numerous bioactive secondary metabolites contain amino acids that are not found in proteins. These unique building blocks may be biosynthesized by discrete pathways or they may be elaborated from the 20 canonical amino acids. The ability of microbes to generate novel amino acids can greatly expand the chemical space and reactivity of natural products and can have a profound effect on biological activity. I will present two studies that are focused on amino acids that are incorporated into bioactive secondary metabolites; the first example involves the biosynthesis of an unnatural amino acid, and the second example is focused on the derivatization of tryptophan.

The nonproteogenic amino acid 3,5-Dihydroxyphenylglycine (DPG) is synthesized and incorporated into the vancomycin family of antibiotics. A key enzyme in this pathway is DpgC, which performs a 4-electron oxidation without the use of metals or cofactors. We studied this unique enzyme using the tools of synthetic organic chemistry, enzymology and structural biology. The structure of DpgC was determined with a bound synthetic inhibitor, which allowed us to identify the active site. We determined the mechanism of DpgC via a systematic study of mutations of catalytically relevant amino acids and alternate substrates.

Lymphostin is a member of the pyrroloquinoline alkaloid family of natural products that contain a tryptophan-derived tricyclic core. Herein we describe the biosynthetic basis of lymphostin production in the marine microbe Salinispora. This pathway involves a uniquely organized polyketide synthase-nonribosomal peptide synthetase hybrid, which incorporates a modified tryptophan that originates from a precursor peptide. We are using a variety of genetic and biochemical techniques to elucidate the method in which this microbe extracts, modifies, and incorporates this amino acid into the final natural product. The knowledge gained from this study can lead to the discovery of pathways for the larger class of pyrroloquinoline alkaloids, which have primarily been extracted from marine sponges or mushrooms.
Chemical tools for the selective detection of phosphorylated proteins

Kathleen C. A. Garber¹, garber@indiana.edu, Erin E. Carlson¹². (1) Department of Chemistry, Indiana University, Bloomington, IN 47405, United States (2) Department of Molecular and Cellular Biochemistry, Indiana University, Bloomington, IN 47405, United States

Protein phosphorylation is a ubiquitous posttranslational modification that regulates cell signaling in both prokaryotes and eukaryotes. The dysregulation of kinases and phosphatases has been linked to many disease processes in humans, including cancer. Accordingly, protein kinases are important drug targets in the pharmaceutical industry. Kinases have recently been identified as potential drug targets in the search for antibacterial agents. Although the study of phosphorylated proteins has made great progress in the last decade, global phosphoproteomics studies are still challenges for several reasons, including the instability of the phospho-amino acid bonds and the low abundance of phosphoproteins. These issues are particularly exacerbated when examining phosphorylation at sites other than Ser, Thr and Tyr. To address these challenges, we are pursuing the development of a chemical method capable of specifically targeting phosphorylated amino acids in order to identify phosphoproteins from complex biological samples.
We present the design and application of a new type of biosensor consisting of two primary components: 1) a small molecule with selectivity for the active state of the target protein, and 2) an environmentally sensitive and membrane permeant dye. The dye was optimized for photophysical properties and uniformity of intracellular distribution and was then conjugated to a chemically modified version of the small molecule in a position that would not interfere with normal binding interactions. The biosensor showed an activation state specific increase in fluorescence intensity upon target binding in vitro of more than tenfold. Subsequent live cell imaging studies showed unique localization of the biosensor signal relative to controls. Current work is focused on exploring the potential of the optimized dyes for in vivo protein labeling and on further application of the small molecule based biosensor approach to other targets of interest.
Progress toward the chemical synthesis of human chorionic gonadotropin β-subunit

Paul A. Vadola, vadolap@mskcc.org, Samuel J. Danishefsky. Department of Molecular Pharmacology and Chemistry, Memorial Sloan-Kettering Cancer Center, New York City, NY 10065, United States

Protein glycosylation is one of the most important and complex post-translational modifications. However, since this process is not strictly regulated the result is often inseparable mixtures of heterogeneous glycoforms of the desired glycoprotein. This inability to isolate homogeneous glycoforms is a major obstacle towards the development of therapeutics. Chemical synthesis obviates this concern, as it offers precise control of molecular structure. We are interested in the use of chemical synthesis as a means to access homogenous forms of complex glycoproteins. Here we will present our progress towards Human Chorionic Gonadotropin (hCG), the primary role of which is the regulation of progesterone and testosterone, with the pendant glycans playing key roles in proper function of the protein. The synthesis we will describe is a convergent approach to hCG that will allow us to easily install an array of desired glycans and investigate their effects on the function of hCG.
Delineating MAPK-substrates interactions using molecular modeling, NMR, and enzyme kinetics

Mangalika Warthaka¹, mangalar@mail.utexas.edu, Sunbae Lee¹, Andrea Piserchio³, Chunli Yan², Tamer Kaoud¹, Ashwini Devkota¹, Ranajeet Ghose³, Pengyu Ren², Kevin N Dalby¹. ¹Division of Medicinal Chemistry, College of Pharmacy, University of Texas at Austin, Austin, TX 78712, United States ²Biomedical Engineering, University of Texas at Austin, Austin, TX 78712, United States ³Department of Chemistry, The City College of New York, New York, New York 10031, United States

The mechanisms by which MAP kinases recognize and phosphorylate substrates are not completely understood. Efforts to understand the mechanisms have been compromised by the lack of MAPK-substrate structures. While MAPK-substrate docking is well established as a viable mechanism for bringing MAPKs and substrates into close proximity the molecular details of how such docking promotes phosphorylation is an unresolved issue. In the present study computer modeling approaches, NMR studies and enzyme kinetics were used to understand ERK2:Substrate interactions as follows: 1) Computer modeling approaches were used to predict how the N-terminus of Ets-1 associates with ERK2. The modeling predicts that the N-terminus of Ets-1 makes important contributions to the stabilization of the complex, but remains largely disordered. The computer-generated model was used to guide mutagenesis experiments, which support the notion that Leu-11 and possibly Ile-13 and Ile-14 of Ets-1 1-138 (Ets) make contributions through binding to the hydrophobic groove of the ERK2 D-recruiting site (DRS). 2) Detailed investigation of the structural perturbations of inactive ERK2 that accompany interactions involving both canonical and noncanonical recruitment events were performed using solution NMR studies. The chemical shift perturbations in inactive ERK2, indicates the structural changes in the presence of canonical and noncanonical motifs, are not restricted to the recruitment sites but also involve the linker that connects the N- and C-lobes. The canonical motifs interact with the DRS utilizing both charge-charge and hydrophobic interactions 3) Two docking interactions mediated peptides were used to understand the coupling of D-recruitment site interactions (DRS) and F-recruitment interactions (FRS). These studies facilitate the potential inhibitor design targeting individual docking interactions of ERK2.
New adventures in structural biology via solid-state NMR

Benjamin J. Wylie¹, bwylie@mac.com, Chad M. Rienstra², Ann E. McDermott¹. (1) Department of Chemistry, Columbia University, New York, New York 10027, United States (2) Department of Chemistry, The University of Illinois Urbana-Champaign, Urbana, IL 61801, United States

Solid-state NMR (SSNMR) is not limited by a sample's solubility or crystallinity, making it ideal to study membrane and fibrillar proteins. SSNMR is also well equipped to measure structurally dependent tensors, including dipoles and anisotropic chemical shifts. We present several recent advances in the field. First, we describe the refinement of model protein structures to atomic resolution using precise tensor measurements. The resulting structures exhibit both precision (~0.16 Å backbone RMSD) and accuracy (~0.5 Å vs. x-ray crystal structure). Next we discuss the spectroscopic characterization of the integral membrane K⁺ channel KcsA using four-dimensional SSNMR. This technique allows key sites of the protein to be resolved despite the high chemical shift degeneracy in largely a-helical proteins. And finally we present advances in the study of membrane proteins using dynamic nuclear polarization (DNP). Specifically, sample preparation techniques will be described that allow systems to be examined under conditions closer to those observed in vivo.
Development of multifunctional biomaterials, which can closely mimic cellular microenvironment and provide necessary signals for cell proliferation, migration, and differentiation, is much needed in the multidisciplinary field of Tissue Engineering. Current strategies involve chemical modifications of the base polymer, which can often change microstructure and chemical composition of the biomaterial, and complicate our understanding of biological responses. We have employed functionalized α-cyclodextrin (α-CD) nanobeads threaded onto the polymer chains that are cell responsive and sensitive to manipulate material properties. With this design, we can enhance cell-material interactions; eliminate variables involved in existing methods, and precisely control material physical and chemical properties. Here we describe the design and synthesis of both α-CD-based hydrogels and electrospun fibers, elucidate structure-property relationships, and demonstrate its applications ranging from stem cell culture and differentiation to tissue regeneration.
Advancing chemistry and interdisciplinary STEM education through interactive simulations, computer-facilitated collaborative chat, and novel instructional strategies

Colin A Ashe¹, colin.a.ashe@gmail.com, David J Yaron¹, W. Craig Carter², Catherine Chase¹, David Adamson¹, Laura Bartolo³. (1) Carnegie Mellon University, Pittsburgh, PA 15213, United States (2) Massachusetts Institute of Technology, Cambridge, MA 02139, United States (3) Kent State University, Kent, OH 44242, United States

I describe a number of recent projects aimed at deepening undergraduate student understanding of difficult and important concepts in chemistry and across STEM disciplines. The longest-running of these projects uses interactive simulations to teach students core concepts related to the behavior of collections of atoms and molecules. These concepts include the energy landscape, entropy, free energy, and how molecular-scale behaviors result in emergent, macroscopically observable properties. Separate investigations are examining the use of an intelligent computer agent to facilitate student discussions about intermolecular forces in a collaborative online chat environment. Additional current studies use a pedagogy based on specially constructed contrasting cases to help students develop a deep understanding of reaction progress and what chemical reaction “equations” mean. Curricular materials and student assessment results will be presented for each project.
Development of a viral nanoparticle for biomedical applications

Michael A Bruckman, mxb588@case.edu. Biomedical Engineering, Case Western Reserve University, Cleveland, OH 44106, United States

I am interested in the development of viral nanoparticles as a nano-sized platform for applications in biomedicine, electronics and sensing. My current training is the development of tobacco mosaic virus (TMV) for imaging atherosclerosis. The use of nanoparticles to diagnose and treat diseases such as cancer and coronary artery disease has shown great potential. The key is to engineer a multifunctional nanoparticle with well-defined properties, i.e. morphology, size, charge, surface ligands for optimal trafficking to sites of disease in vivo. My career has focused on engineering tobacco mosaic virus (TMV), which presents a robust hollow rod-shaped platform capable of undergoing chemical conjugation to its interior and exterior surfaces. TMV is also capable of transforming to RNA-free spherical nanoparticles (SNPs). The size and polydispersity of these SNPs is highly controllable, therefore offering a unique platform to test the effect that shape has on biomedicine.
Understanding and controlling biological structure and self-assembly are critical to problems ranging from treating diseases to engineering hybrid materials for electronic applications. My research has addressed these issues in two complementary ways. The first is by synthesizing and assembling precisely controlled inorganic nanocrystal bioconjugates in which a single biomolecule is attached per nanocrystal. This approach enables controlled assembly of hybrid biological/inorganic materials for plasmonic and enzymatic studies. The other is to image peptide structure directly at the sub-nanometer scale using a custom-built microwave-modulated scanning tunneling microscope. Combined with advanced image analysis techniques and large-scale semi-empirical molecular models, this approach provides early steps toward analyzing protein structure at the single-molecule level without requiring crystallization.
Colloidal particle synthesis, DNA zipper based springs, and drug delivery capsules that deliver their payload upon detection of a specific DNA sequence

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Metallic hallow nano-bowls were synthesized, fitted with a DNA zipper based spring mechanism and a colloidal lid capping the bowl. Upon interaction with specific DNA strands the nano-bowl and lid complex disassociated delivering their internal payloads. A DNA zipper is a double-stranded DNA system engineered to open upon specific interaction with an appropriately designed single strand DNA. The opening of the zippers is driven by binding energy differences between the DNA strands. The zippers were incorporated with defined modifications to function like a spring and are capable of delivering ~9 pN of force. The kinetics of the system was studied and model of their interaction is presented.
Design, synthesis, and assembly of nanoscale building blocks for hierarchical structured functional materials

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Development of functional materials having hierarchical structures across multiple length scale with a single particle precision (< 5 nm) is current challenge in nanotechnology. Future technologies dependant on the devices integrated with building blocks with built-in functionalities that exhibit biological, optical, electronic or magnetic properties, which are responsiveness to the external stimuli or extremely selective to the exposed environment. The key requirement to achieve this includes designing building blocks, understanding principles governing self-assembly, and implementation to direct the assemblies precisely at various length scales. More specifically my research will be focused on a) synthesis of organic-inorganic hybrid nanostructured materials using colloidal approach, b) develop methodologies to control its short and long range interactions c) develop stimuli-responsive systems d) generate hierarchical structures at multiple length scales and explore the collective properties. This will generate novel optical metamaterials for applications including advancement of photovoltaics, solar-cells, as well as smart biosensing devices.
Controlling surface properties of metal oxide nanoparticles using polymer brushes

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Recently, there has been much interest in polymer film modification onto semiconductor nanoparticles due to their efficiency in tunable wavelength light emission, which has led to increased application of luminescent nanoparticles making their study very intriguing. For such purposes, controlling the surface functionalization is important and can be tailored by the attachment of organic acids via self-assembled monolayers (SAMs). In this study, metal oxide nanoparticles (ZnO and SiO₂) were modified using SAMs with phosphonic acid functional groups. Furthermore, polymers were grafted onto the surface by surface-initiated free radical polymerization (SIP) using azo-initiators and SAM as the platform for in situ formation and attachment. The polymer brushes were formed by using styrene, Bis[2-(methacryloyloxy)ethyl] phosphate, and 4-Allyloxy-2-hydroxybenzophenone. The modified nanoparticles were then characterized using infrared spectroscopy (IR), solid-state nuclear magnetic resonance spectroscopy (SS-NMR), powder X-ray diffraction (PXRD), and scanning electron microscopy (SEM). The band gap was calculated for the modified nanoparticles.
Recent experiments demonstrate that the lanthanides have an active reduction chemistry with species such as N$_2$, NO, CO and CO$_2$, and that complexes of unprecedented radical species, such as (N$_2$)$^{3-}$ and (NO)$^{2-}$ can be isolated.$^{1,2}$ To elucidate the nature of the metal valence orbitals involved in these reactions and products, density functional theory calculations were performed for a series of La, Ce, Sm, Dy, Ho, Er, and Y compounds. We present results for structures, IR spectra, and UV/Vis spectra all indicating the 5d orbitals play a much larger role in the reduction chemistry of rare-earth compounds than previously expected. In particular, we report computational studies on the first molecular examples of Ho(II) and Er(II), as well as photochemically active [C$_5$Me$_5$]$_2$(C$_4$Me$_4$H)Ln complexes.


High performance computational investigations of Stone-Wales defects and reactivity in single-walled carbon nanotubes: Applications toward hydrogen storage and sensors

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Currently, I am a post-doctoral research associate with Prof. Jerzy Leszczynski at Jackson State University. I have four years of teaching experience, over 40 peer-reviewed publications, and 6 book chapters. I have more than 50 presentations in the form of posters, and oral (few invited talks). I have an h-index of 14.

The formation energy of single Stone-Wales (SW) defect with possible two different orientations in (5,5) single-walled carbon nanotubes (SWCNTs) has been investigated using ab initio and DFT methods. Our study reveals that a 90 degree rotation of an axial C-C bond is slightly more preferred than the circumferential C-C bond in forming the Stone-Wales defect. The reactivities of various carbon sites on (5,5) SWCNT of C$_{70}$H$_{20}$ with and without the Stone-Wales defect have been predicted. Our study indicates that chemisorptions of one and two hydrogen atoms on the external surface of (3,3), (4,4), (5,5) and (6,6) armchair SWCNTs are exothermic processes. We found that two hydrogen atoms favor to bind at adjacent positions and the exothermicity of hydrogen chemisorptions decreases while the diameter of armchair nanotubes increases.
New approach to biological simulations

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We study central enzymes of cellular energy generating system by computer modeling of molecular dynamics. The common bio-molecular models, however, are not reliable in all solvation conditions relevant to physiological processes. To resolve this critical issue we have invented a number of novel algorithms and developed a new computational concept [1] of Molecular Dynamics in Electronic Continuum (MDEC). The new technique, as shown by different authors, significantly extends the range of problems that can be studied within the computationally efficient non-polarizable models. In simulations of the enzyme Cytochrome c oxidase the approach gives rise to new qualitative results in respect to the traditional methods. I have published about 20 peer-reviewed publications on this subject summarized in our recent review [1].

Implicit solvent calculations with explicit molecular models in amber with 3D-RISM

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Physiologically relevant modeling of biomolecules requires the accurate inclusion of solvation effects. Explicit solvent molecular dynamics provides this but at considerable computational cost. Continuum implicit solvation methods are fast but ignore the discrete, molecular nature of water and require extensive parameterization. In contrast, the 3D-reference interaction site model (3D-RISM) uses statistical mechanics to calculate the equilibrium properties of common explicit-solvent models, including water and co-solvents, around biomolecules of arbitrary shape and size. Here we provide an overview of 3D-RISM and its implementation in the Amber molecular modeling suite. 3D-RISM's capabilities are illustrated using three examples: calculation of the free energy of protein-ligand binding in biotin-avidin complex, the ionic atmosphere around a 24-base pair DNA duplex and the role of hydration in cucurbit[7]uril host-guest system.
In vivo protein biophysics: Insights from novel theoretical and computational approaches

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Understanding and manipulating protein folding and protein homeostasis in living cells is one of the great challenges facing this generation of biophysicists. It requires that we understand the concomitant folding of proteins during their biosynthesis by the ribosome molecular machine, a factor shown to be important in determining the cellular concentration of successfully folded proteins. I will discuss my efforts to understand the physical principles of such co-translational folding through the development of coarse-grained simulation force-fields, chemical kinetic modeling, and systems biology methods. I will show how these tools have allowed us to gain novel insights into fundamental issues of in vivo folding, including the impact of variable translation rates and synonymous codon usage, the effect of chaperones, and, at the cellular level, the co-translational folding properties of the E. coli proteome under different growth conditions. These methods are opening up new avenues of research in the areas of synthetic biology, biotechnology and biomedicine, where, for example, they potentially provide a framework for rationally redesigning transcriptomes to yield cells with desirable proteostasis properties.
Development and application of computational methods to biological and technological systems

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My research work has been focused in the study of macromolecules, and smaller molecules with biological interest and technological applications. Many aspects of my research were centered on systems with transition metal complexes, as they have particular computational requirements, and are important in catalysis, materials synthesis, photochemistry, and biological systems. The methodologies that I applied in my research range from pure Molecular Mechanics (MM), to pure ab initio, including hybrid QM/MM methods. At the ab initio level, I devised methodologies to evaluate the effect of stereoelectronic interactions on molecular properties. At the pure MM level, I developed force field (FF) methodologies to account for dihedral energy coupling in amide foldamers, and applied it to Molecular Dynamics (MD) simulations. At the QM/MM level, I collaborated in the development of Moving-Domain QM/MM methods, which allow the computation of properties of macromolecules of biological relevance, at the equivalent of a QM level.

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

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Presented is a time line of a project dedicated to manufacture polymers that will enhance uptake of uranium from seawater as compared to the existing polymer technology. The first principles analysis of a single amidoxime functional group revealed a correct binding motif to uranyl cation. Molecular dynamics modeling of existing amidoxime polymers revealed amidoxime-carboxylate pair as a ligand responsible for binding uranyl. Computer aided design yielded covalently linked bis-amidoxime ligand as the ultimate chelating ligand. Solvation modeling yielded sulfonate as the most practical group to help expose ligand to the seawater and sustain harsh chemical conditions during metal elution process. Finally, two amidoxime groups covalently connected and derivatized with sulfonate and attached to polymer was synthesized and tested for affinity toward uranyl cation in seawater.
Developing methods of computational chemistry and biology

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We have worked more than ten years in the areas of computational chemistry and biology including the areas of quantum chemistry, molecular dynamics simulation and computer-aided drug design, to develop methods and apply these methods to chemical bonding, nano-size structures, metal clusters, enzyme activation mode, protein structure determination, protein-protein and protein-ligand interactions including drug design. We are planning to further develop the relevant methods to a wide range of application areas.
There are many technologies for soil and water remediation, and my research seeks to develop efficient and cost-effective nanotechnology-enabled physico-chemical treatment of emerging contaminants such as pharmaceuticals (estrogen hormones), organic contaminants (polycyclic aromatic hydrocarbons (PAHs), dyes and polychlorinated biphenyls (PCBs)), inorganic contaminants (Cr(VI) and lead), metalloids (arsenic) and emerging contaminants (1,2,3-Trichloropropane). In particular, my research interests include 1) investigation of physico-chemical treatment combined with Advanced Oxidation Process (AOP) for contaminant remediation, 2) investigation of the fate and transport of nanomaterials and their fundamental treatment mechanism, 3) utilization of industrial byproducts for contaminants solidification/stabilization.
Characterizing air mass collected at lower troposphere (<2 km) during the 2011 student airborne mission (SARP): Focused on the high frequency sampling during the missed-approach to LAX

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During the NASA Student Airborne Program (SARP) mission, high frequency whole air sampling during a missed-approach to Los Angeles International airport (LAX) provided air mass signatures collected in close proximity to their urban and oceanic sources. Each whole air sample was analyzed for 80 speciated halocarbons, hydrocarbons and organic nitrates. Unlike other airborne missions, high frequency whole air sampling of about 70 samples collected over a 20 minute period (15 second fill per sample) during a 150 km flight path at low altitude (< 2 km) provided a more detailed profile of the Los Angeles air shed than has been previously possible. Correlations between CH₃I, CHBr₃, and MeONO₂ (marine tracers) versus C₂Cl₄ and HCFC-22 (anthropogenic tracers) were used to distinguish between purely marine air and air influenced by emissions from Los Angeles.
Of the 80 speciated C$_1$-C$_{10}$ volatile organic compounds that were measured, 60 were elevated in air from the Los Angeles air shed. These included C$_1$-C$_{10}$ alkanes, C$_6$-C$_8$ aromatics, C$_2$-C$_3$ alkenes, halons, HCFCs, HFCs, CH$_3$CCl$_3$, chlorinated solvents (e.g., C$_2$Cl$_4$, CHCl$_3$, CH$_2$Cl$_2$), and organic nitrates. Marine species emitted in this region of the Pacific were found to include MeONO$_2$, EtONO$_2$, CH$_2$Br$_2$, CHBr$_3$, CH$_3$I and DMS. Note that the C$_3$ organic nitrates were not enhanced in the marine wing, and instead they are attributed to urban photochemistry. Overall, high-frequency and low-altitude whole air sampling during the LAX missed-approach clearly distinguished urban and oceanic sources and allowed a detailed chemical signature for Los Angeles air to be determined.
Nanoscale hybrid materials for sustainability

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Through my graduate and post-doctoral research in chemistry and materials science and engineering, I developed expertise in nano-scale materials for environmental applications with emphases on gas separation and carbon capture, utilization and storage.

My PhD work focused on the design and tuning of reactive carbon-based adsorbents for the gas separation of small molecules, with identification of the effect of the adsorbents' physical and chemical features. Part of this research led to the development of metal-organic framework/graphite oxide composites exhibiting among the best ammonia adsorption capacities reported so far (patented work). My post-doctoral research entails the synthesis, characterization, and evaluation of nano-scale inorganic-organic hybrid materials for CO₂ capture/conversion and H₂ production from biomass. I plan to focus my academic career on the development of nanoscale and waste-derived materials in the crosslinking areas of water and energy sustainability.
Analyzing post combustion CO\textsubscript{2} capture solvent degradation products

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My current research focuses on identifying and quantifying degradation products from post combustion CO\textsubscript{2} capture solvents at a pilot CO\textsubscript{2} scrubber and stripper unit. A significant problem with using chemical adsorption of CO\textsubscript{2} with amine-based solvents is the degradation through irreversible side reactions with CO\textsubscript{2} and other flue gas components. Numerous problems can exist in this process including loss of the amine solvent, formation of ammonia, aldehydes, corrosive acids, hazardous nitramines and nitrosamines, and finally the disposal of these hazardous chemicals leading to increased disposal costs. We have been performing extensive analytical testing of both liquid solvent and flue gas samples using IC, GC/MS, HPLC and LC-TOF-MS to examine possible degradation pathways and develop strategies to minimize production of these degradation products and the likelihood of adverse human and environmental impacts they may cause.

My previous research centered on developing analytical methods to characterize sustainable biofuel feedstocks using a variety of techniques and instrumentation including headspace solid phase microextraction (HS-SPME), GC/MS, GC/FID, Spray desorption collection (SDC), HPLC and LC/MS and Mass Spectrometry. I also developed human sensory evaluation protocols to evaluate biofuel feedstocks and worked on a project to formulate life-cycle assessment parameters used to evaluate the sustainability and commercialization of alternative biofuel feedstocks.
New idea in source apportionment analysis: A combination of iterative updating algorithm with eigenspace projection

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Traditional source apportionment analysis can be distinguished into two categories: 1. Pure mathematical iterative updating method aim for minimizing the difference between measured data matrix and reconstructed data matrix. 2. A geometric approach which identify sources through determining the edges and/or vertices of the measurements in a multidimensional eigenspace. The pure algorithm method has inherent shortcoming due to matrix rotation, while the geometric method suffers from large data uncertainty. A new approach is showing here firstly using the eigenspace projection to properly determine number of factors and to eliminate the effect of data rotation, then a mild matrix updating technique is applied to find the optimized solutions.
Catalytic processes for the production of biobased chemicals and petrochemicals from renewable feedstocks

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

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The identification and understanding of the coordination, electronic structure and reactivity of catalytic intermediates is quite important for developing the streamline of chemical syntheses in making useful pharmaceutical, organic materials or even fuels. The author will present her graduate research work from Georgetown University that involved the unraveling of an efficient copper(I) catalyzed C-H bond amination via the study of the electronic structures and reactivity of metal-nitrene intermediates. Postdoctoral research at Johns Hopkins extends her quest for the fundamental understanding of mechanistic catalytic pathways to the oxidation of biologically relevant iron-sulfur sites. Cysteine Dioxygenase is an enzyme that is vital in human metabolic processes that uses oxygen and a three histidine iron(II) site to catalyze the oxidation of cysteine to cysteine sulfinic acid. Non-heme iron(II) thiolate models were synthesized and the mechanism of oxygen activation was investigated. She is currently an active team member in the artificial photosynthesis group at Brookhaven National Laboratory in the field of solar energy research working on understanding proton-coupled electron (PCET) processes of ruthenium(II) water oxidation catalysts. Future research plans will target the design of catalysts relevant to artificial photosynthesis and the activation of small molecules for the understanding of metalloenzyme functions.

The work at Brookhaven National Laboratory (BNL) is funded under contract DE-AC02-98CH10886 and the work at Houston is funded under contract DE-FG02-07ER15888 with the U.S. Department of Energy and supported by its Division of Chemical Sciences, Geosciences, & Biosciences, Office of Basic Energy Sciences. The BNL authors also thank the U.S Department of Energy for funding under the BES Hydrogen Fuel Initiative.
Experimental and computational methods for the deconstruction and valorization of lignin

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Lignin is among the most abundant natural heteropolymers on Earth. While lignin represents an abundant feedstock material for the production of renewable fuels and value-added chemicals, it is an underutilized value stream in current biomass conversion technologies because there exist no economic and technically feasible routes for lignin depolymerization and upgrading. My work at NREL has focused on elucidating deconstruction pathways of this recalcitrant polymer using homogeneous and heterogeneous catalysts. This entails testing putative catalyst species against a library of model compounds as well as using computational modeling of the substrates and catalysts to determine thermodynamic and kinetic parameters. From these preliminary studies, I hope to develop strategies for the selective conversion of biomass to fuels and chemicals. Synthetic techniques applicable to a model compound library, synthesis and spectroscopic characterization of catalyst species, as well as DFT studies of all of the aforementioned will be presented.
Nature has perfected the synthesis of inorganic materials and organic-inorganic architectures in aqueous environments and under mild physiological conditions. We use M13 bacteriophage, or phage, to harness the power nature has over interactions between proteins or peptides and inorganic materials. Through peptide phage display, we have identified a library of short peptide sequences with specificity for inorganic materials, which we refer to as specific peptides. These specific peptides have been used to develop a technique to magnetically separate target nanomaterials from solutions containing a mixture of nanomaterials. In addition, we have exploited nonspecific interactions of surface peptides with metal salts to create nanoarchitectures of phage decorated with metal nanoparticles. We have also developed a room-temperature aqueous method to synthesize nanoparticles of the metastable alloys Au-Rh, Au-Pt, Pt-Rh, and Pd-Rh, which we can anchor to phage to reduce agglomeration.
Bulk-heterojunction materials for photovoltaics: Synthesis and exploration of novel routes for semiconductor nanostructures and polythiophene - polyselenophene derivatives

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The synthesis and characterization of bulk-heterojunctions of novel materials that are relevant to solar energy conversion is presented. A novel synthetic route using adamantane derivatives of sulfur and selenium is used to achieve new materials at significantly more benign chemical conditions. The synthesis and characterization of semiconductor nanostructures of ZnS, CdS, ZnSe, and CdSe was achieved using these adamantane derivatives at lower temperatures than published methods.

. The synthesis and characterization of polythiophene and polyselenophene molecules was achieved using a nanoCuO catalyst route. The charge transport properties of our new materials were tested to determine their feasibility for bulk-heterojunctions.
Functional supramolecular constructs of edge-binding phthalocyanines and porphyrins, and of the bridging ligand 1,6,7,12-tetraazaperylene

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As an accomplished, award-winning chemistry educator who has successfully taught inorganic, organic, analytical, and advanced synthesis chemistry and supervised synthesis research at the undergraduate and graduate level, I would bring a quality level of teaching, research and outreach to your department. My teaching experience also includes the special courses "Science Fiction Science", teaching the science and writing of science fiction; "Life with the Atom", about nuclear technology in our society; and “Exploring Materials Science”, for first-year chemistry students. My current research program at Gustavus Adolphus College enlists six students exploring the goal of incorporating phthalocyanines, porphyrins and the bridging heterocyclic ligand 1,6,7,12-tetraazaperylene into functional supramolecular structures for potential electronic, catalytic, nanotechnology and biomedicine applications. Pedagogical techniques for helping students develop an excitement for chemistry will be discussed. [Ph.D., Chemistry: Univ. Illinois; postdoctoral: Univ. Minnesota, Univ. Iowa; teaching: Grinnell Coll. (Adjunct), Tennessee State Univ., Muhlenberg Coll., Gustavus Adolphus Coll. (Adjunct, current)]
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Using general chemistry concepts in cutting edge catalytic transformations and energy research

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The concept of Lewis acids and bases presented in general chemistry has been reinvigorated in the current chemical literature with the recent discovery of “frustrated Lewis pairs.” This concept, using non-interacting Lewis acids and bases, exhibits unique and unexpected chemistry. This AEI Poster will describe how this fundamental general chemistry concept of Lewis acid/base chemistry can be used in the development and understanding in the current research areas of catalytic H₂, O₂, and N₂ activation and their energy related transformations.
Inorganic nanomaterials: Functional scaffold in therapeutics and diagnostics

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The past decade has shown tremendous advances in the synthesis of inorganic nanomaterials with precisely controlled structures and properties. If we can engineer these nanomaterials to sensitively diagnose cancer and infectious diseases, it will provide critical information for stratifying patients and assessing treatment efficacy. Furthermore, the development of nanomaterials for drug delivery will improve the bioavailability and enhance the therapeutic efficiency. My research efforts in functional inorganic nanomaterials have focused on 1) the synthesis of highly porous nanomaterials as versatile carrier and delivery system for biologically active molecules, and 2) the development of signal amplification in magnetic resonance assay for point-of-care cellular diagnostic. These efforts are specifically designed to address two issues: How can we provide relevant clinical diagnoses using limited sample specimen and minimal purification? How can we enhance the therapeutic efficacy to eliminate the disease, but minimize the damage to healthy tissues? Combining these methods with current technology can potentially resolve current diagnostic and therapeutic challenges in oncology and global health.
Half-sandwich Fe electrocatalysts for H₂ oxidation and production

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By taking advantage of the well-designed diphosphine ligands (P₂N₂) that feature built-in amines as proton replays, a series of half-sandwich Fe complexes supported by these functional chelating phosphine ligands have been developed as effective molecular electrocatalysts for H₂ oxidation and H₂ production. Specifically, [F₅PhCpFe(P²Bu₂N²Bn₂)H], [F₄PyCpFe(P²Bu₂N²BtBu₂)H] and [F₄PyCpFe(P²Bu₂N²tBu₂)H] (where F₅PhCp is perfluorophenylcyclopentadiene anion ligand, F₄PyCp is tetrafluoropyridinylcyclopentadiene anion ligand, P²Bu₂N²Bn₂ is 1,5-terbutyl-3,7-dibenzyl-1,5-diaza-3,7-diphosphacyclooctane and P²Bu₂N²tBu₂ is 1,5-terbutyl-3,7-terbutyl-1,5-diaza-3,7-diphosphacyclooctane) are demonstrated to be the first examples of Fe-based electrocatalysts for catalytic H₂ oxidation with turnover frequencies (TOFs) as high as 2.5 s⁻¹ and overpotential as low as 100 mV. These molecules also function as fast electrocatalysts for catalytic H₂ production (TOFs as high as 365 s⁻¹) employing weak acids.
Amyloids and copper biochemistry: Effects of metal dyshomeostasis in Alzheimer's and Parkinson's disease

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Copper is a vital biological element that is essential for human health, however, the same characteristics that make this metal important also make it detrimental if not controlled. In order to maintain proper metal storage and delivery, a complex regulatory system exists. An alteration in this homeostasis can trigger oxidative stress due to aberrant redox chemistry or abnormal metal-protein interactions. In fact, metal dyshomeostasis with age is thought to contribute to Alzheimer's disease (AD) and Parkinson's disease (PD) pathologies. One aspect of the presented research will focus on AD related vascular inflammation potentially caused by copper-bound amyloid-β peptide (CuAβ) and the associated production of reactive-oxygen-species (ROS). Vascular damage due to CuAβ toxicity could lead to inefficient oxygen delivery followed by mild cognitive impairment and eventual neurodegeneration. Furthermore, experiments supporting copper promoted α-synuclein misfolding and aggregation as a result of protein oxidation, as implicated in PD, will also be discussed.
Chiral and achiral Cu(II) and Ni(II) complexes with novel multidentate ligands

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Tetradentate and hexadentate ligands, with N4 and S2N4 donor sets respectively, were complexed with Cu(II) and Ni(II) to form chiral and achiral chelates. The tetradentate ligands were prepared using vinylpyridine and chiral piperazine derivatives to form both enantiomers of the chiral complexes, as well as similar non-chiral mono and dinuclear complexes using achiral derivatives of piperazine and homopiperazine. The hexadentate ligands were synthesized from 2-hyrazinopyridine and alkyl and aryl bridged dithio-diketo precursors, which were prepared using either a N,N,N-triethyl-N-(propan-2-onyl)ammonium or N,N,N-triethyl-N-(phenylethan-2-onyl)ammonium chloride salt and a range of dithiols. Crystal structures and absorption data will be presented as well as ECD plots for the chiral complexes and magnetic data for the dinuclear complex. Complexes were also characterized using electrochemistry and ESR.
Catalyst development on the molecular and nano scales

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Catalyst development, with applications ranging from pharmaceutical and fine chemicals to energy, is a major component of harnessing the benefits of chemistry now and into the future. Therefore it is important to pursue any and all catalysts, homogeneous and heterogeneous, molecular and nanoscale, to accomplish a desired reaction. This poster will highlight efforts to develop catalysts in two veins. The first is progress toward a homogeneous, molecular catalyst for conversion of natural gas into liquid fuels, a process dominated by use of heterogeneous catalysts. The second is design of colloidal nanomaterial catalysts for organic synthesis, an area where molecular catalysts are traditionally employed.
Synthesis and reactivity of transition-metal catalysts for main group bond forming reactions

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Bond-forming reactions represent one of the best, atom economical routes to produce new, synthetically valuable compounds. As a graduate student at the University of Vermont my research involved the synthesis and characterization of early-metal zirconium complexes that were able to catalyze bond-forming reactions of phosphorus. I was able to work with several graduate, undergraduate, and high school students with this project.

As a postdoctoral researcher at the University of San Diego, I have focused on using easily accessible organometallic complexes to facilitate organic reactions involving boron. This included selective C-H borylation reactions of benzylic amines by iridium complexes. The interdisciplinary nature of this research between organic and inorganic chemistry is ideal for undergraduate students interested in a career in chemistry and will be the focus of my research group as an independent faculty member. During my time as a postdoctoral researcher I was also the primary instructor organic chemistry II lecture. Teaching this class has highlighted and enhanced my desire to become an independent faculty member at a primarily undergraduate institution.
Development of novel therapeutics, combinations, and formulations of photodynamic therapy agents for the treatment of cancers

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My research interests lie at the intersection of biological, medicinal and inorganic photo-chemistry. The focus of my doctoral work involved the synthesis, characterization and photophysical study of a series of Ru(II) polypyridine complexes as potential photoactivated anti-tumor agents. These complexes were applied to a burgeoning field of medicine known as photodynamic therapy (PDT), where, after undergoing a photoinduced ligand exchange, these complexes have light induced cytotoxicity similar mode of action to the cancer drug cisplatin. Furthermore, I spearheaded the development of a cross functional team at The Ohio State University Medical Center working closely with surgeons, pharmacists and engineers to develop the bioconjugation and testing of an immunoguided fluorescence intraoperative imaging probe. This antibody conjugate was used to improve sensitivity and resection margins of current oncological detection techniques. My Ph.D. work therefore laid a solid foundation for an approach to science as an interdisciplinary endeavor, working across the boundaries within and beyond the field of chemistry.

Currently, I am continuing to explore an interdisciplinary approach to scientific research as a Harvard Medical School Research Fellow in the laboratory of Dr. Tayyaba Hasan at Massachusetts General Hospital. At MGH, I have expanded my experience in biology by designing, synthesizing and characterizing liposome and bio-polymer based formulations of FDA approved PDT agents and biological therapeutics. In experiments in vivo using (orthotopic model of pancreatic cancer), the fully formulated liposomes were shown to significantly reduce tumor burden by as much as 80% when compared to unformulated individual drug components given in combination or as monotherapies. As a result of this work, I have learned valuable concepts of biology, techniques of nanotechnology formulation and shared my chemistry background to develop new liposomal drug formulations.
Synthetic organometallic chemistry offers undergraduate students opportunities to learn both synthetic skills and characterization techniques which can be used a variety of post-graduate contexts. This poster presents both the development of molecular frameworks from aromatic hydrocarbon complexes of \{\text{TpW(NO)(PMe3)}\} and the NMR and electrochemical techniques that are indispensable in guiding their synthesis. Though many of the reactions presented are straightforward organic reactions, the products they generate are substantially different from those generated in traditional organic chemistry. We use 2D NMR techniques, X-ray crystallography, and HRMS to determine the structure and stereochemistry of our organic products. Isolating the new organic molecule from the metal complex requires use of cyclic voltammetry to choose appropriate oxidants. Additionally, incorporation of computational techniques has given us insight into experimental observations of reactivity and stereoselectivity.
Interrupting bacterial communication: The design and synthesis of small molecules for quorum sensing regulation

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*Pseudomonas aeruginosa* is a strain of bacteria responsible for thousands of deaths of immuno-compromised patients a year, and exhibits a high capacity for antibiotic resistance. Overcoming antibacterial resistance requires exploring novel mechanisms of action such as intercellular bacterial communication, termed quorum sensing (QS). QS is a population-density-dependent process where bacteria use a set of chemical signals called autoinducers to coordinate behaviors of a population. Specifically, QS in *P. aeruginosa* is used to activate pathogenic traits.

The proposed research involves an investigation into the synthesis and activity of small molecules designed as regulators of QS in *P. aeruginosa*. A small molecule library will be synthesized based on variations of a structurally distinct compound set known as the triphenyl compounds which have similar receptor binding to the natural autoinducer. A structure activity relationship will be used to determine the effect of each small molecule on QS activity, and adjustments to the structure will be made accordingly.
Pancreatic cancer is the fourth leading cause of cancer related deaths in the U.S. Most patients with the disease are treated with a combination of surgery, chemotherapy and/or radiotherapy. The five year survival rate after diagnosis is less than five percent. Currently, one of the main hurdles in transitioning of these drug delivery systems to the clinic has been sequestrerization of the nanoparticles by the reticuloendothelial system. This results in the accumulation of the diagnostic and/or therapeutic agents in non-target tissues such as the liver and spleen leading to toxicity. Taking advantage of the presence of cysteine cathepsins proteases, we developed cleavable peptide linkers that can increase non-target clearance while still yielding high tumor retention thus increasing the efficacy of radiolabeled diagnostic and therapeutic polymer based agents for pancreatic cancer.

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The first single step regioselective formation of diazadioxacalix[4]arenes and diazadioxa[1,4]cyclophanes is described. These macrocycles were formed via condensation of 3- or 4- amino-phenols, with 1,5-difluoro-2,4-dinitrobenzene. Conformational properties of the macrocycles, as well as the mechanistic details leading to the observed bridging pattern where investigated.
Synthesis and biological evaluation of natural product-like macrocycles containing integral carbohydrate moieties

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Natural product-like molecules containing a macrocycle are attractive synthetic targets due to their novel molecular architectures. Additionally, they often present biological activity. Previous efforts from our group delivered carbohydrate-fused [11.4.0] macro-dilactones. We also prepared macrolactones that are fused through the C1 and C5 positions of a pyranose ring. The connectivity to the carbohydrate affords a [n.3.1] bicyclic system. The novel macrolactones have been produced via a concise synthetic sequence that includes acylation of a 1-allyl glycoside followed by ring closing metathesis (RCM). [12], [13] and [14] member lactones which contain an alkene have been produced. Structural investigations of the new macrocycles including crystallographic data have been obtained. Presentation of mild antibiotic activity has prompted diversification at C4 of the [9.3.1] pyranose system to develop a biological profile of the new targets.
Tungsten catalyzed heterocycloisomerizations and the total synthesis of diterpenoid alkaloids

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The development of a W(CO)₅ catalyzed heterocycloisomerization of bicyclo[4.1.0] substrates to form substituted 4,5-dihydrobenzofurans and dihydroindoles is presented. These heterocycles show reactivity that is orthogonal to that of the corresponding benzofurans and indoles. 4,5-Dihydrobenzofurans and dihydroindoles are versatile intermediates for the synthesis of various natural products.

Additionally, progress toward the total synthesis of the diterpenoid alkaloid cossonidine is shown. This approach utilizes a hydrindanone intermediate that we believe will allow for diversification and access to a number of diterpenoid alkaloids.
How to teach anything to anyone while increasing enrollment and learning in general and organic chemistry and solving student retention, solar energy, skin cancer, and Alzheimer's with undergraduate research

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**Teaching**: Experienced, excellent communicator and popular Organic and General Chemistry teacher with innovative educational ideas: I increased classroom enrollment in parallel credit classes by as much as 10 times the normal enrollment as a professor. Class sizes taught: 50 to 300 students. Excellent teaching evaluations by students, colleagues and deans. Experience teaching a wide variety of students (95% white, 85% African American, 30% hispanic, first generation economically disadvantaged, honor's, military related students). **Research**: My ongoing research projects (as principal investigator) from my former faculty position will continue. (Project-applications) (1) Biomimetic materials: DNA and chlorophyll functionalized carbon nanotubes - solar energy, semiconductors (2) Photodimerization of thymine – understanding skin cancer. (3) Stereoselective synthesis of tropanes using the zwitterionic effect and organoaluminum catalysis – potential pharmaceuticals for neurobiological diseases like Parkinson's & Alzheimers. (4) Educational research project is training students with limited scientific back to do research efficiently and quickly. [http://JulietHahn.com](http://JulietHahn.com) Drop by to chat.
Influence of varied polymer and end group moieties on the self-assembly and nanoscale architecture of Poly(3-hexylthiophene) materials

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The ability to control self-assembly in nano-structured materials plays a prevalent role towards the development of highly optimal electronic devices. As such, the self-assembled components can strongly affect the internal processes associated with energy transfer and conversion in semiconductor devices. In addressing this issue, directed self-assembly can provide a route to well-organized structures with high molecular level precision and minimal structural defects that have been proven detrimental to organic electronic applications. Controlling the supramolecular self-assembly via molecular composition and functionality offers a unique strategy to provide targeted functional patterns in a reproducibly controlled fashion. As such, the incorporation of other polymers or end groups via copolymerization and/or organic syntheses to induce various idealized morphologies towards the design of efficient and high-performance electronic devices will be investigated. Herein, I demonstrate the use of copolymerization and end group functionalization procedures to influence the intrinsic properties poly-3-alkylthiophenes. P3HT block copolymers consisting of various units will be discussed in terms of their structure-property relationships with distinct focus on the influence on self-assembly and electronic properties of P3HTs.
Electrophilic cyclization: Application in synthesis of biologically important heterocycles

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Iodocyclization is a process in which an internal alkyne tethered to a nucleophile can undergo a ring forming reaction in the presence of molecular iodine. In past decade iodocyclization reactions have emerged as a powerful tool for the synthesis of a wide variety of heterocycles. This method has been successfully employed in the synthesis of benzo[b]selenophenes, thiophenes, benzopyrans, pyridine and pyrroloquinoline. Simple staring compounds, mild reaction conditions and ease in product isolation make these methodologies very useful. Palladium-catalyzed cross coupling reactions were employed to functionalize these core structures in order to form some biologically interesting analogues. In future these reactions could be used to synthesize porous materials for H₂ storage and catalysis. They could also be very useful method for combinatorial and green chemistry.
Self-assembly and fibrillar structures of molecular gels derived from (R)-12-hydroxystearic acid as gelator

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(R)-12-Hydroxystearic acid ((R)-HSA) can be isolated in large amounts from castor oil. Our research shows that amine and amide derivatives of (R)-HSA, in which alkyl chains of different lengths are appended to the nitrogen atom of an amine or amide, gelate efficiently a wide variety of organic liquids at room temperature.\[1\] Organogels formed from (R)-12-hydroxystearamide as gelator recover a large part of their viscoelasticity within seconds of being destroyed by excessive shearing; they are thixotropic.\[1\] This recovery is an order of magnitude faster than any other organogel with a crystalline fibrillar network reported to date. In other study, an unprecedented thermally-reversible gel-gel phase transition was observed for the CCl4 gel phases of some of the amine derivatives of (R)-HSA. These unexpected first-order phase transitions have been characterized using spectroscopic, diffraction, thermal and rheological techniques. IR and SANS data are consistent with the expulsion (on heating) or the inclusion (on cooling) of molecules of CCl4 that are between the bundled fibers.\[2\] We also report that several of N-alkyl-(R)-12 hydroxyoctadecylammonium chlorides, the hydrochloride salts of the amines, are efficient ambidextrous gelators (gelating both water and a variety of organic liquids), needing less than ca. 0.5 wt % at room temperature.\[3\] The self-assembled fibrillar networks of the hydro- and organo-gels of the N-alkyl-(R)-12 hydroxyoctadecylammonium chlorides have been explored in detail. These gelators provide a versatile platform for probing fundamental questions regarding the links between molecular structure and one-dimensional self-aggregation, as well as approaches for the design of new materials, such as thixotropic gels.\[4\]

We thank the National Science Foundation for its support of this research.


From single molecule to device: Building a better understanding of structure-property relationships in organic solar cells, field effect transistors, and molecule-based electronics

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Organic based electronics are lighter, more flexible, and considerably less expensive than their inorganic counterparts. Despite these desirable properties, many organic electronic devices are limited by their performance. For instance, organic solar cells are cheap to manufacture, yet currently provide less than 10% solar conversion efficiency. However, with a deeper understanding of the fundamental electrical and physical properties of molecules, high performance organic electronics can be realized through careful synthetic design and improved device processing. The work presented here represents a breadth of organic electronics research including: 1) a novel patterning technique used to investigate the electrical properties of molecules by forming nano-scale metal electrodes on top self-assembled monolayers, 2) the development of new materials for high-performance organic photovoltaics and field effect transistors, and 3) the study of the structure-property dynamics between molecule design and device performance.
Synthesis of alpha-hydroxy ketones and aldehydes via the dioxygenation of vinyl boronic acids

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Aldehydes and ketones that have oxygen substituents at the alpha-position are important building blocks for the synthesis of a large number of biologically active compounds. Conventional transformations which afford the alpha-oxygenation products of carbonyl compounds either utilize oxidants that are unstable or involve the removal of halogenated byproducts after displacement with oxygen nucleophiles. We have developed a new alternative route to alpha-oxygenated carbonyl compounds through the dioxygenation of vinyl boronic acids which avoids the use of unstable reagents, undesirable side-products and provides a direct route from internal alkynes to alpha-oxygenated ketones. The use of N-hydroxyphthalimide to afford the dioxygenation of vinyl boronic acids will be presented: a two-step procedure involving the copper-catalyzed etherification of N-hydroxy phthalimide with boronic acids and a subsequent [3,3] rearrangement of the N-enoxypthalimide coupling products will be described. The stereoselectivity of the rearrangement to form the alpha-oxygenated ketones and aldehydes as well as simple procedures for the cleavage of the alpha-imidate products to give alpha-hydroxy ketones in good yields will also be discussed.
Controlling recruitment of transcriptional complexes with bifunctional small molecules

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Nuclear receptors (NRs), such as glucocorticoid receptor (GR), are ligand-inducible transcription factors that regulate gene expression by recruiting protein complexes to DNA. NRs are important therapeutic targets which, historically, are modulated with small molecules that allosterically recruit transcription cofactors. However, this regulatory pathway collapses in many diseases with mutated NRs. Alternatively, bifunctional small molecules that can directly control cofactor recruitment would provide an alternative pathway for regulation. As a proof of principle, a collection of bifunctional molecules were designed, synthesized and used to recruit the potent transcriptional activator VP16 to GR. VP16 recruitment results in higher levels of transcriptional activation than classical GR agonists and can completely override the intrinsic function of classical GR antagonists. We are currently exploring bifunctional ligands containing histone deacetylase (HDAC) inhibitors to recruit endogenous transcriptional corepressors. My independent career will focus on the discovery of new chemical ligands for these and other histone modifying cofactors.
Better living through quantum chemistry

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My scientific goals focus on gaining a comprehensive understanding of the dynamical behaviour of molecular systems. Fundamental chemical and biological processes, from solar energy harvesting to protein regulation, involve the simultaneous rearrangement of both electrons and nuclei. Accurate simulation of these interacting particles will reveal information about the quantum mechanical nature of matter at the molecular level. The principle research strategies I employ include cutting-edge quantum chemical computational techniques as well as analytical theory.
Predictive molecular simulations of nucleation phenomena and phase equilibria

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Computer simulation has become an increasingly valuable tool that can use molecular level information to predict properties on the meso and macroscales and can provide valuable insight into how molecular properties give rise to these behaviors. This work will describe recent advances in the development of computational tools for simulations of nucleation processes and phase equilibria and several applications of these tools including: (i) an investigation of the nucleation processes controlling the formation of atmospheric aerosols, which currently represent the main source for uncertainties in global climate models, (ii) a computational design of solvent-based ethanol extraction systems for the large-scale separation of ethanol from fermentation broths, which would eliminate the need for energy-intensive distillation for the use of ethanol as a transportation fuel and chemical feedstock, and (iii) the development of accurate force fields for hydrofluorocarbons that are being considered as alternative refrigerants.
Predictive and fast: New tools for first-principles catalyst and enzyme design

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Rational, computational design is a promising pathway to the development of novel catalysts, enzymes, and materials, but the effectiveness of this design strategy is dependent upon the predictive accuracy and computational cost of the methods employed. Density-functional theory (DFT) is a widely-employed approach for determining the electronic structure of molecules and solids, but standard DFT suffers from a critical error known as self-interaction that yields erroneous descriptions of geometry and energetics. By augmenting standard DFT with a system-dependent Hubbard term, my methods achieve a level of accuracy that provides insights into the tethered catalysis activity of a halogenase relevant for natural product synthesis, new strategies for carbon capture catalyst design, and predictive descriptions of chemisorption on surfaces. Additionally, my recent work in accelerated quantum chemistry on novel architectures enables the determination of the electronic structure for systems thousands of atoms in size, paving the way for new enzyme and drug design.
Nonlinear laser spectroscopy used as a molecular probe

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Laser spectroscopy is a powerful tool, both in analytical and physical chemistry. It can be used to identify molecular structure, investigate molecule-surface interfaces, and probe the electronic structure of molecules. I have routinely used many types of laser spectroscopy, coupled with quantum mechanical studies, to explore the complex nature of various probe molecules. My research has focused mainly on surface enhanced hyper Raman spectroscopy (SEHRS), an optical probe of nonlinear vibrational scattering processes. By utilizing nonlinear spectroscopy, I can access molecular transitions which are classically forbidden in linear optical processes. This is a superior technique because it utilizes wavelengths that are transparent to biological tissue. I have also run experiments that show surface enhancements in SEHRS can produce signal from extremely low concentrations, which may lead to single molecule detection. My poster will also display the work I have done in developing laboratories for General Chemistry courses.
Nonequilibrium thermodynamics of biomolecular machines

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I am a biophysical chemist who uses theory and computational techniques to study the nonequilibrium thermodynamics of molecular-scale biological processes. My research program focuses on questions where non-equilibrium statistical mechanics and information theory provide ground-breaking insights into the fluctuation-dominated behavior of biomolecular systems. Through my research I intend to uncover the basic principles of driven biomolecular-scale energy conversion, especially the physical constraints placed on biomolecular machines by their operational imperatives: doing useful work in finite time while driven by strong gradients in the fluctuation-dominated microscopic realm of a cell at room temperature. Such insights into the constraints on efficient nanoscale energy conversion may illuminate efforts to devise therapeutics for the numerous human illnesses (including cardiomyopathy, neurodegeneration and cancer) resulting from the dysfunction of particular biomolecular machines. Design principles derived from these constraints should also prove useful in synthesizing artificial molecular machines, for example for solar energy conversion or drug delivery.
Spectroscopic and computational approaches to understanding enzyme regulation: Connecting large-amplitude vibrations in small molecules to allosteric activation

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Chemical reactivity is fundamentally linked to distortion of a molecule away from its equilibrium geometry. In small molecules, the pathways connecting isomeric minima correspond to large-amplitude vibrations. Displacements along these coordinates have the capacity to distort the electronic wavefunction, reflected in changes in experimentally observable properties.

The conformational landscape of an enzyme is vastly more complicated. Allosteric effectors modulate the ensemble of protein conformations, favoring or disfavoring reaction-competent geometries. Mechanistic understanding of the catalyzed reaction informs spectroscopic observables characterizing the enzyme active site.

I use computational docking to identify candidate small-molecule allosteric effectors of enzyme activity from a metabolite library. Docking hits are screened for binding by NMR, and tested for allosteric action by monitoring changes in the chosen spectroscopic quantities. This approach will identify potential connections between biochemical networks and shed light on the biochemical context of enzymes of unknown function.
Surface-specific vibrational lineshapes with subwavenumber resolution: Influence of the spectroscopic phase in coherent nonlinear spectroscopy

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The ability of surface vibrational spectroscopy for revealing molecular structure and dynamics is often limited by the presence of overlapping bands and low instrumental resolution. Here, a unique approach for rapidly obtaining the broad-bandwidth surface vibrational spectra with sub-wavenumber resolution is to be presented. The information revealed by the high-quality band envelopes allows for interface-specific conformational and interaction details to be determined at an unprecedented level of resolution. The frequency-domain lineshapes are directly compared with their corresponding time-resolved curves providing highly consistent information. In addition, the polarization analysis of the sum-frequency signal proves to be crucial for the spectroscopic phase to be used as an anchoring parameter for the unambiguous determination of unresolved spectral features which are only 2-10 cm\(^{-1}\) apart. In this way, detailed interfacial structure and molecular interactions can be quantitatively obtained as demonstrated here for various liquid and solid interfaces of atmospherical, biological, or technological relevance.
Selenoamino acids and the development of biomaterials responsive to reactive oxygen species (ROS)

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Oxidative stress is a common biological effect resulting from the imbalance of reactive oxygen species (ROS) generated and depleted in living organisms. This disruption in oxidative species can result in widespread cellular damage with systematic physiological consequences often associated with tissue injury and disease. Herein, we describe methodology that takes advantage of the unique reactivity of selenium-based amino acids to undergo oxidative elimination to form alkenes and subsequent conjugate addition with thiols. We exploit this reactivity to develop elastin-based biomaterials that are responsive to reactive oxygen species. We demonstrate this transformation in cross-linked gels and hydrogels, and discuss its application in ROS dosimetry and drug delivery. This research outlines a strategy by our laboratory to utilize artificial amino acids to introduce novel reactivity and structural properties in proteins.

The oxidation of selenium compounds to promote unique reactivity in biomaterials serves as a platform for my future research interests in introducing small, oxidized molecules (i.e. SO₂ and CO₂) into organic molecules. This ongoing work compliments my previous research experience in metal catalysis and mechanism. An aspect of my future research will focus on the development of green strategies using metal catalysis to convert biomaterials such as lignin and cellulose to common energy and industrial feedstocks.
Hygro-responsive membranes for effective oil-water separation

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There is a critical need for new energy-efficient solutions to separate oil-water mixtures, especially those stabilized by surfactants. Traditional membrane-based separation technologies are energy-intensive and further limited, either by fouling or the inability of a single membrane to separate all types of oil-water mixtures (i.e., free oil and water, oil-in-water emulsions, water-in-oil emulsions and any combination of these phases). The ideal membrane for solely gravity-driven separation of oil-water mixtures is expected to be both hydrophilic and oleophobic, in air and under water. Recently (Nature, 2012, in press), we have developed superhydrophilic (i.e., water contact angles $\sim 0^\circ$) and superoleophobic (i.e., oil contact angles $> 150^\circ$) that allow us to separate all types of oil-water mixtures solely using gravity in a single unit operation, with $> 99.9\%$ separation efficiency.
Multifunctional nanomaterials are extensively investigated for promising applications both in energy and biomedical research. My cross disciplinary research training at UNT gave me excellent experience and skills on syntheses, characterization and knowledge of different types of materials; luminescent molecules/nanoparticles, metallic nanoparticles (Au, Ag, Cu, Au-Ag), stimuli sensitive hydrogels (PNIPAM, Chitosan, PEG), polymeric nanoparticles and hybrids (luminescent polymeric nanoparticles, polymers interfaced luminescent systems) derived by interfacing these different material systems. Though started with focus on syntheses but significance of these hybrid materials for broad spectrum of applications has initiated fabrication and testing of these materials for imaging, sensing and detection studies. Considering biological importance, invitro, invivo and antipathogenic studies have shown considerably improved features compared to analogues known in literature.
Macromolecular nanoengineering: Fabrication and characterization of polymer based nanostructures

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My research interests span the designing of soft materials (polymer and colloids) for (i) electronic cooling, (ii) energy conversion/storage and (iii) sensing applications.

During my graduate work, I studied the effect of ion beam irradiation on the structural, thermal and electrical properties of PET, PVC and composites of PVC with a conducting polymer polyaniline. We demonstrated the role of polymer backbone on its stability under extreme environment and also established that a controlled radiation dose can improve the polymer properties. As a post-doc at Georgia Tech, I have explored the adsorption and interaction of charged (polymer) colloid particles at oil-water interface in different solvent conditions and particles' stabilized emulsions. We also studied the surfactant mediated charging of colloid particles and charge screening in non-polar solvents. Currently, I am working on electrochemical fabrication of conjugated polymer nanostructures for thermal interface applications.

As an independent researcher, I would like to establish a research program on design and fabrication of polymer-based nanosystems for energy storage, separation and sensing applications. I am experienced and capable of teaching at undergraduate and graduate levels. The courses I would be interested in teaching include, but are not limited to, physical chemistry, analytical chemistry, instrumental methods of chemical analysis, polymer characterization and processing, bio-physical chemistry, colloid & surface chemistry, nanomaterial fabrication & characterization and electrochemistry.
Noninvasive optical imaging to investigate the passive distribution of polymeric nanocarriers in vivo

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Noninvasive optical imaging was used to assess the distribution of polymeric nanocarriers in tumor and retention in breast ducts. The PEG polymers of different molecular weights were labeled with a fluorescent dye and administered intravenously to female balb/c mice bearing subcutaneous 4T1 tumors. The tumor distributions were measured noninvasively using an In Vivo Imaging System. The polymers exhibited selective distribution in tumor, compared to other organs, and the tumor distribution increased with increasing molecular weights. The same method was used to measure the retention of intraductally-administered polymers in the breast duct of female Sprague-Dawley rats. The ductal retention of polymers increased with increasing molecular weights. In a parallel work, MRI was used to measure the surface coverage, retention, and degradation of vaginal hydrogels for microbicide delivery. The noninvasive imaging is advantageous because it provides a reliable and rapid method for the initial screening of polymer distribution and pharmacokinetics.
Bottom-up synthesis of graphene nanoribbons from poly(\(p\)-phenylene-ethynylene)

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Graphene nanoribbons (GNR) are nanostructured fragments of single-layer graphene in which one of the sizes much longer than the other and possible two edge structures. Dictated by their edge structure, GNRs can perform as metals or semiconductors with great potential in the field of nanoelectronic devices. This work comprises the preparation of GNRs via chemical modification of polymers, achieving control in their metrics, edge features, presence of heteroatoms, and processability. The synthetic strategy used was a two-step sequence starting from easily synthesizable poly-(1,4-phenylene-ethynylene) polymers with varying solubilizing side chains and high molecular weight. Newly developed cycloaddition reactions transform the alkyne of the polymer into naphthalene units with very high conversions forming poly(1,4-phenylene-2,3-naphthylene) followed by the intramolecular oxidative C-C coupling of the polymer afforded GNR in high yields. Depending on the nature of the side chains of the initial polymer, GNRs could be prepared with hydrophobic alkyl and hydrophilic oligo-ethylene-oxide side chains, and their effect on the dispersability in organic solvents and water was explored. The GNRs were characterized by size-exclusion chromatography, photoabsorption, photoemission, infrared, Raman, and nuclear magnetic resonance spectroscopies, thermal gravimetry and imaging.
Self-assembly of ferritin around gold nanoparticles

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Thermophilic ferritin (tF) from the hyperthermophilic archaeon, *A. fulgidus*, was found to encapsulate 5- or 10-nm gold nanoparticles (AuNPs). Incubation of tF with 5- or 10-nm AuNPs in low-salt buffer initiates a self-assembly process that incorporates the AuNP within the ferritin cavity. Experimental data support that tF maintains wild-type stoichiometry and structure in these bio-nano conjugates. Significantly, tF-NP conjugates template the growth of larger NPs. Stable bio-nano conjugates with templating abilities can be used in many biomedical applications including targeting or imaging.
Chitosan nanoparticles for time-released delivery of oxytocin: Applications in autism treatment

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Chitosan nanoparticles (CSNPs) have been extensively investigated for delivering peptides to the animal brain and have shown great potential for therapeutic applications. In this study, we prepared oxytocin-loaded chitosan nanoparticles proposing extended hormone release in the brain for autism treatment. Oxytocin-loaded CSNPs were formed spontaneously using ionotropic gelation with tripolyphosphate (TPP). Structure, morphology, stability, size, and size distribution of the synthesized nanoparticles was studied by various analytical techniques including scanning electron microscopy (SEM), transmission electron microscopy (TEM), confocal laser scanning microscopy (CLSM), X-ray diffraction (XRD), LC/MS, thermogravimetric analysis (TGA), nanoUV, and Fourier transform infrared (FT-IR) spectrometer. Our results suggest that CS-OXY nanoparticles can have a great potential in mouse model systems.
Mutagenesis: From molecular mechanisms to biomarkers

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DNA is prone to attack by physical and chemical agents generated endogenously and exogenously, producing modified DNA bases (i.e. DNA adducts or lesions), abasic sites, and DNA-DNA and DNA-protein cross-links. DNA adducts, if not properly repaired, can lead to blocked replication, misincorporation, and mutation, potentially causing cancer and other diseases. My research interests center on understanding the replication and repair of DNA modification (postdoctoral training), and developing novel methodologies to detect DNA lesion as disease biomarkers (Ph.D. thesis). Recent accomplished projects include: (1) understanding the DNA polymerase (replicative and translesion) replication pattern of \( N^2,3\)-ethenoguanine(G), an important DNA lesion resulting from exposure to vinyl chloride or from lipid peroxidation. We successfully utilized a 2'-fluoroarabinose strategy to stabilize this well-known labile lesion. A series of biochemical and crystallographic studies reveal the major mutation as T pairing with \( N^2,3\)-ethenoG. Project (2) involves synthesis of DNA-protein cross-links and investigation of their mutagenesis potential. Major experimental approaches are chemical synthesis, steady-state kinetics, liquid chromatography-mass spectrometry and X-ray crystallography.