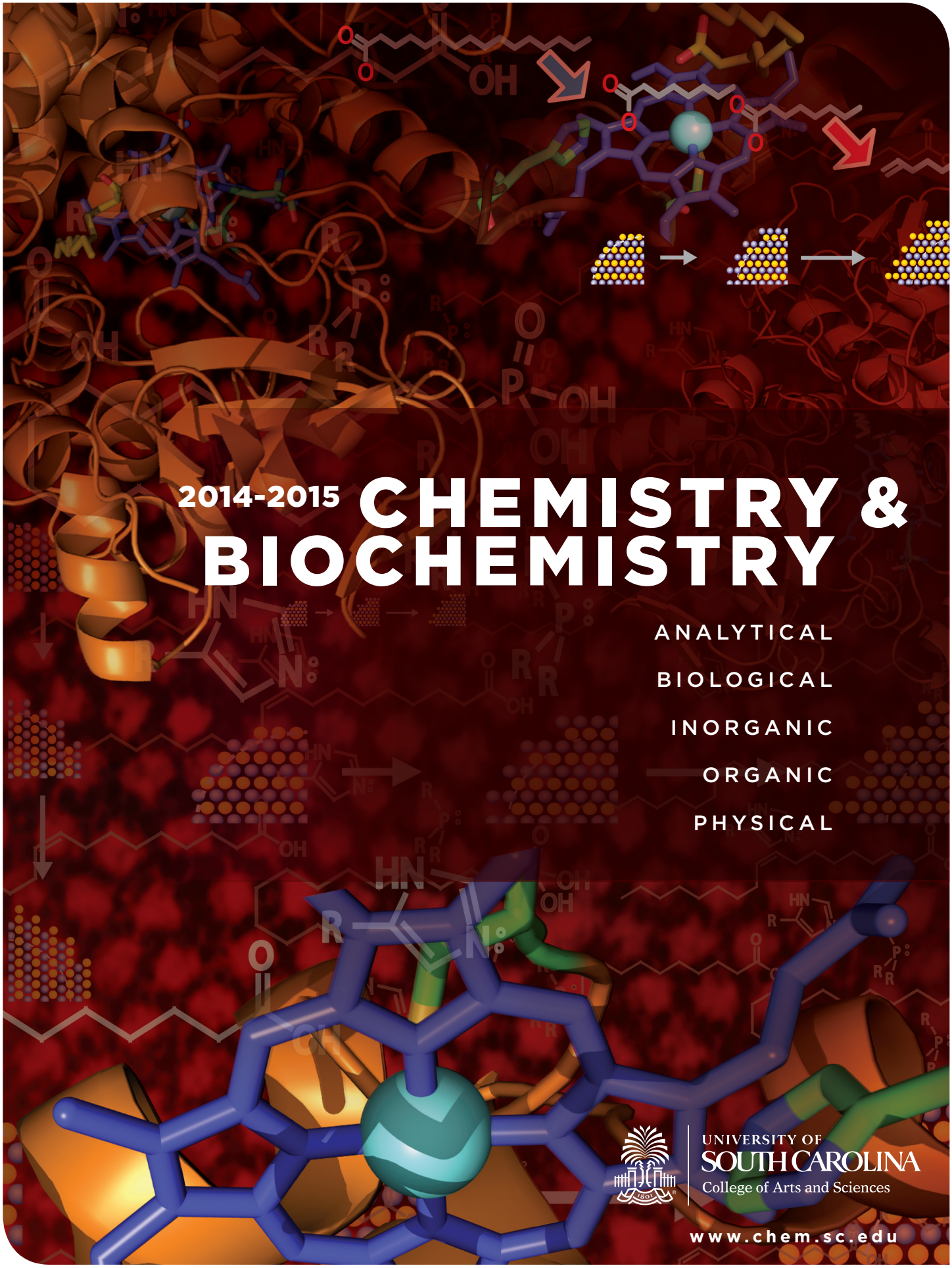

2014-2015

CHEMISTRY & BIOCHEMISTRY

ANALYTICAL

BIOLOGICAL

INORGANIC

ORGANIC

PHYSICAL

UNIVERSITY OF SOUTH CAROLINA
College of Arts and Sciences

www.chem.sc.edu

DEPARTMENT HIGHLIGHTS

PEOPLE

- We maintain a friendly and highly collaborative research environment.
- We currently have 35 active research faculty members, 29 postdoctoral and other senior researchers, 144 graduate students, and 24 staff members.

RESEARCH

- In the most recently updated NRC ranking of chemistry programs calculated at Cornell University, we ranked #25 nationally based on a composite average of quality indicators, such as the number of publications per faculty member, the number of citations received per publication, the percentage of faculty with research funding, and the number of times faculty have been recognized with significant awards.
- The National Science Foundtion regularly ranks USC in the top 35 in Chemistry departments in the national in total spending far outperforming most institutions of comparable size.
- We publish approximately 160 research papers every year.

FACILITIES

- We occupy the $36-million John M. Palms Center for Graduate Science Research, dedicated in 2000.
- Research facilities include the Nuclear Magnetic Resonance Center, the Mass Spectrometry Laboratory, the X-ray Diffraction Facility, and the College of Arts and Sciences Stockroom. The Electron Microscopy Center is located in an adjacent building.

LOCATION

- Columbia is one of the nation's "10 most livable mid-sized cities" according to the Partnership for Livable Communities, with a metro area population of more than 700,000.
- Kayaking, boating, hiking, and bicycling are popular outdoor pastimes. Metropolitan Columbia has three major rivers running through it and has been listed as one of the top 10 canoe towns in the country by Paddler Magazine.

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COVER

Features the alternating layer addition processes that control the growth of core/shell quantum dot nanoparticles from Dr. Greytak's group. Dr. Makris group's investigation of several P450 enzymes that catalyze the oxidative decarboxylation of long chain fatty acids to alkanes or alkenes, which enable the production of biomass-derived fuels via engineered microbial pathways. The image was designed by Prof. Greytak, Prof. Makris, and Jemimah Ekeh and features research by graduate students Rui Tan and Job Grant.

THE UNIVERSITY OF SOUTH CAROLINA

Chartered in 1801 as South Carolina College, the University of South Carolina was the first state university supported continuously by annual state appropriations. By the 1850s, it had achieved a reputation as one of the best endowed and most distinguished colleges in the United States. Hard hit by the Civil War and Reconstruction, the school struggled for many years to survive.

Its renaissance as a modern university began in the 1950s. Since then, dynamic academic expansion has produced highly diverse and innovative educational programs. A commitment to graduate education and involvement in major research initiatives have attracted an outstanding faculty. Today, in addition to the Columbia campus, the University includes seven other campuses around the state. Enrollment on all campuses totals more than 47,000. Of these, more than 32,000 students are on the Columbia campus, about one-third of whom are enrolled in graduate and professional programs.

The University offers myriad degree programs, including master's degrees in 111 areas, Ph.D. degrees in 64 fields, and first-professional degrees in law, medicine, and pharmacy. Many programs are nationally and internationally ranked. More than 1,800 master's degrees and about 320 Ph.D. degrees are awarded annually. The graduate students make up more than 27% of the total student body at USC Columbia.

USC libraries hold more than 8 million items. The Thomas Cooper Library, the main campus library, seats about 2,500 readers and features study rooms, seminar rooms, computer labs, and individual lockable carrels for researchers. An integrated computer information system allows access to holdings from any computer terminal. Its newest addition, the Ernest F. Hollings Special Collections Library, opened in summer 2010. It houses South Carolina Political Collections, the Irvin Department of Rare Books and Special Collections, and Digital Collections. There are separate libraries for medicine, law, mathematics, music, and business.

In addition to extensive faculty and graduate student research conducted through various academic departments, the University operates several permanently established research facilities, including the Belle W. Baruch Institute for Marine and Coastal Sciences, the Institute for Public Service and Policy Research, the Earth Sciences and Resources Institute, the S.C. Institute of Archaeology and Anthropology, and the Richard L. Walker Institute of International and Area Studies. Grants of more than $328 million were received in fiscal year 2013 in support of research and other sponsored programs at the University.

In keeping with both its 19th-century and 20th-century heritage, the University continues to promote academic excellence. USC has committed itself to earning a place among the finest institutions of higher learning in America. Such ambitions and ideals were cornerstones of the original college and remain fundamental to the University of South Carolina today.

DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY

The Department of Chemistry and Biochemistry began offering a research-oriented Master of Science degree in 1948. In 1954 the graduate program was expanded to include the Doctor of Philosophy. Since then the graduate research effort has broadened and intensified. Today the department counts 144 graduate students, about 24 postdoctoral fellows, and 35 full-time faculty members.

The department's staff includes three undergraduate laboratory supervisors, a full-time staff crystallographer, several technicians and operators in the biochemical instrumentation core facilities, and four staff scientists in the NMR and Mass Spectrometry laboratories. In addition, the department has access to the College of Arts and Sciences machine shop and the USC Electron Microscopy Center.

The quality and promise of the graduate program in chemistry and biochemistry has been recognized outside the University as well as within. Twenty-four times in the past 56 years the University of South Carolina's Russell and Educational Foundation Research Awards for Science, Mathematics, and Engineering have gone to a member of the chemistry and biochemistry faculty. Six faculty members have been named research fellows of the Alfred P. Sloan Foundation, and five faculty members have won the University's highest honor for excellence in teaching, the Amoco Foundation Award. The University's Michael J. Mungo Award for Excellence in Undergraduate Teaching has been won by nine faculty members from our department. Our biochemistry faculty have joint appointments with the School of Medicine; eight have received that school's Basic Science Research Award. Our faculty have also received national and international recognition from American Chemical Society awards and by serving as editors and editorial advisory board members for prestigious chemical journals. Eight faculty members from the department have received the Governor's Award for Excellence in Science, awarded annually to the top research scientist in the state of South Carolina. Since its inception in 2005, three faculty members from the department have received the Governor's Award for Scientific Awareness and for excellence in science.

The department continues to hire and develop outstanding new faculty. New hires recently made include biochemistry faculty Drs. Maksymilian Chruszcz, Thomas Makris, and Mythreye Karthikeyan, as well as analytical/environmental faculty Dr. Susan D. Richardson, Professor and Arthur Sease Williams Professor of Chemistry. Inorganic faculty Drs. Dmitry Peryshkov, and Natalia Shustova and organic faculty member Dr. Morgan Stefik joined the department in summer 2013. Our newest faculty member, Dr. Aaron Vannucci, joined the department in inorganic chemistry in the summer of 2014.

THE GRADUATE PROGRAM IN CHEMISTRY AND BIOCHEMISTRY

The Department of Chemistry and Biochemistry offers a graduate program leading to the Doctor of Philosophy with concentrations in analytical, biological, inorganic, organic, and physical chemistry. The course and research requirements are flexible and can be tailored to the background and interests of each student. Multidisciplinary areas such as nanoscience, environmental science, materials science, and optics/spectroscopy are well-represented in the department. Collaborative research between research groups is encouraged.

Advanced degree programs in the department are designed to produce skilled, broadly educated, and creative scientists. While students will concentrate their studies and research in a particular specialty area, it is the philosophy of our department that all students should receive a well-rounded, graduate-level education in several areas of chemistry. Specialization in a particular area, coupled with advanced training in other areas, provides our graduates with flexibility and a broad base of knowledge from which to tackle research problems.

ADMISSION REQUIREMENTS

Prospective graduate students should complete a baccalaureate program that includes one year each of general chemistry, organic chemistry, calculus-based physical chemistry, and analytical chemistry (one-half year instrumental). Given the diverse background of many of our faculty, applications from students from allied programs in the molecular sciences are also strongly encouraged. All components, including a final transcript acknowledging the degree, are required for admission to the graduate program. Additional course work in inorganic and biological chemistry may be helpful.

The general portion of the Graduate Record Examination (GRE) is required for admission. The GRE advanced chemistry scores are not required, but are encouraged, especially for students with an interest in additional fellowships.

THE PH.D. PROGRAM

FIRST YEAR: You and your faculty advisors will work out a program of study appropriate to your background, interests, and abilities, taking into consideration your performance on the qualifying examinations (taken prior to registration). First-year students take five advanced graduate courses (three in the major area) during the first two semesters. All required Ph.D.-level course work is normally completed by the end of the second semester. You must maintain a grade point average of "B" or better in order to continue beyond the first year. A foreign language is not required.

In August and September of your first year, you will attend seminars in which each faculty member makes a brief presentation about his or her research. These seminars will help you select a research director and a lab group to join. You may choose your research director in mid-November; at the latest, you must join a lab group by the first day of your second semester.

By the end of your first academic year, you must qualify in two of the five areas of graduate-level chemistry (analytical, biological, inorganic, organic, and physical), either by passing the qualifying examination or by receiving a grade of "B" or better in a designated qualifying course. One of the two areas must be your major area of interest.

All summers in the program are dedicated to research.

SECOND YEAR: Early in your third semester, you will write and orally defend a report describing progress to date on a research project and your plans for continuing the project. Successful completion of the report satisfies The Graduate School's requirement for an oral comprehensive exam.

During your fourth or fifth semester, you will write and orally defend a proposal focusing on an original research idea. Satisfactory performance on the proposal meets The Graduate School's requirement for a written comprehensive exam.

COMPLETION OF THE PROGRAM: After completing the proposal, the faculty will evaluate your overall academic record to determine whether you may continue as a Ph.D. candidate. Once you have been admitted to candidacy, you will continue your research and prepare your thesis.

Candidates for the Ph.D. are required to present three seminars during the course of their thesis studies. The last of these is the thesis defense; the earlier seminars are on literature or research topics.

Our graduate students currently average a little less than 4 and a half years to complete the Ph.D. program.

PH.D. TASKS BY SEMESTER

SEMESTER	1	2	3	4	5	6	7	8	9
GRADUATE CLASSES	■	■							
TEACHING ASSISTANTSHIPS	■	■							
CHOOSE ADVISOR	■								
CONDUCT RESEARCH		■	■	■	■	■	■	■	■
LITERATURE SEMINAR		■							
RESEARCH PLAN			■	◪	◪				
RESEARCH PROPOSAL				◪	◪				
PH.D. CANDIDACY									
DIVISIONAL SEMINAR					■				
PH.D. THESIS DEFENSE									■

SHENGFANG SUN (BIOCHEMISTRY)

RESEARCH ADVISOR: DR. JOHN H. DAWSON

FIRST YEAR
Took four graduate courses: Biological Chemistry, Structural and Functional Nucleic Acid, Research in Microbiology and Immunobiology and Topics in Advanced Neural Cell

SECOND YEAR
Presented a biochemistry divisional seminar (fall): *Dehaloperoxidase (DHP)* and *Notomastus chloroperoxidase (NCPO): globins with catalytic functions*

FIFTH YEAR
Poster presentation at the Oakwood Products Graduate Student Poster Competition
2014 Outstanding Dissertation Award, USC Graduate School

AFTER GRADUATION
Postdoctoral Fellow at the Florida State University, in the lab of Dr. Hong Li (Department of Chemistry and Biochemistry)

FACTS:

FIRST YEAR

- Teaching assistant for Fundamental Chemistry (fall)
- Rotations in the lab of Dr. Qian Wang (fall) and Dr. John H. Dawson (spring)
- Selected Dr. John H. Dawson as research advisor and began research (spring)

SECOND YEAR

- Took one graduate course: Introduction to Crystallography
- Passed oral comprehensive and research plan (spring)*: Structural and functional studies of Amphitrite Ornata dehaloperoxidase that has dual physiological roles*
- Collaborated with the lab of Dr. Daping Fan (University of South Carolina Medical School) on the project of "A new recombinant human apolipoprotein E mimetic peptide"

THIRD YEAR

- Teaching assistant for General Chemistry (spring)
- Passed written comprehensive and original research proposal (fall): *Identification of intracellular proteins interacting with PCSK9: implications in the mechanism of PCSK9-mediated LDLR degradation*
- Presented a biochemistry divisional seminar (spring): S*tructural and functional studies of Amphitrite Ornata dehaloperoxidase that has dual physiological roles*

FOURTH YEAR

- Awarded J.R. During Graduate Student Travel Award
- Poster presentations at the 18th International Conference on Cytochrome P450, Seattle, Washington
- Teaching assistant for General Chemistry (spring)
- Collaborated with the lab of Dr. Rajagopalan Bhaskaran (Claflin University) on the project of "NMR discovery of the substrate binding site of *Dehaloperoxidase (DHP)*"

FIFTH YEAR

- Teaching assistant for General Chemistry (spring)
- Oral presentation at the USC Graduate Student Day
- Wrote and defended Ph.D. dissertation: *Insights into the evolutional adaptations and functional switching mechanism in dual function hemoglobin/dehaloperoxidase (DHP)*

REPRESENTATIVE PUBLICATIONS

"Mono-and bis-phosphine-ligated H93G myoglobin: Spectral models for ferrous-phosphine and ferrous-CO cytochrome P450" *J. Inorg. Biochem.* 2013. 127, 238-245.

"Complexes of dual-function hemoglobin/dehaloperoxidase with substrate 2, 4, 6-trichlorophenol are inhibitory and indicate binding of halophenol to compound I" *Biochemistry*. 2013. 6203-6210.

"Influence of heme environment structure on dioxygen affinity for the dual function Amphitrite ornata hemoglobin/dehaloperoxidase. Insights into the evolutional structure–function adaptations" *Arch. Biochem. Biophys*. 2014. 545, 108-115.

"Evidence for direct involvement of substrate TCP radical in functional switching from oxyferrous O_2 carrier to ferric peroxidase in the dual function hemoglobin/dehaloperoxidase from *Amphitrite ornata" Biochemistry*. 2014. in press.

JAMES MAZZUCA(PHYSICAL)

RESEARCH ADVISOR: DR. SOPHYA GARASHCHUK

SUMMER BEFORE FIRST YEAR
Copenhaver Fellow under Professor Vitaly Rassolov

SECOND YEAR
Poster presentation at the Second Annual EPSCoR Conference; Served as a judge at the USC Science and Engineering Fair (also 3rd and 5th year)

FIFTH YEAR
Received the Lipscomb Award for the poster/talk "Modeling enzymatic proton transfer with quantum trajectories" at the USC Graduate Symposium

AFTER GRADUATION

Accepted position as Assistant Professor with the Department of Chemistry at Alma College in Alma, MI.

FACTS:

FIRST YEAR

- Joined Prof. Sophya Garashchuk's research group
- Teaching assistant in physical chemistry lab (fall) and honors general chemistry lab (spring)
- Provided free tutoring to undergraduate physical chemistry students (all 5 years)
- Took five graduate-level classes: Quantum Chemistry, Spectroscopy and Molecular Structure, Biosynthesis of Macromolecules, Statistical Mechanics, Multiscale Modeling

SECOND YEAR

- Passed oral and written comprehensive research plan (fall): Trajectory study of quantum effects of nuclear motion in proton transfer reactions
- Passed oral and written original research proposal (spring): Modeling through-space electron transfer in aqueous solution with a time-dependent wavepacket approach
- Spent the summer at Oak Ridge National Lab for research collaboration

THIRD YEAR

- Took a graduate level math course: Computational Math II
- Presented a physical chemistry divisional seminar: Description of proton transfer in soybean lipoxygenase-1 employing approximate quantum trajectory dynamics
- Poster presentation at SETCA 2012
- Participated in the USC Chemistry Outreach program (also 4th year)
- Attended a winter workshop: Theory Winter School: Computational Approaches for Electronic/Magnetic Materials
- Attended a summer workshop: VSCE Programming Heterogeneous Parallel Computing Systems

FOURTH YEAR

- Presented at the organic chemistry summer seminar series: Description of proton transfer in soybean lipoxygenase-1 employing approximate quantum trajectory dynamics
- Awarded a travel grant to present a poster at the conference: Advances in Quantum Chemistry: Interfacing Electronic Structure with Dynamics
- Teaching assistant for undergraduate physical chemistry lecture and recitation (spring)
- Mentored a high school student through the SPRI program
- Contributed talk at SETCA 2013: Description of proton transfer in soybean lipoxygenase-1 employing approximate quantum trajectory dynamics

FIFTH YEAR

- Developed a new experiment which has been implemented in the undergraduate physical chemistry lab at USC
- Mentored an undergraduate student in the Magellan Scholar research program
- Contributed talk at the APS national conference: QTES-DFTB dynamics study on the effect of substrate motion on quantum proton transfer in soybean lipoxygenase-1
- Wrote and defended dissertation: Approximate Quantum Trajectory Method for Modeling Chemical Reaction Dynamics: Application to Enzymatic Proton Transfer

REPRESENTATIVE PUBLICATIONS

L. Wang, J. W. Mazzuca, S. Garashchuk, and J. Jakowski. The hybrid Quantum Trajectory/Electronic Structure DFTB-based approach to Molecular Dynamics. Paper presented at XSEDE14 Annual Conference, 2014.

J. Mazzuca, S. Garashchuk, and J. Jakowski. Description of proton transfer in soybean lipoxygenase-1 employing approximate quantum trajectory dynamics. *Chem. Phys. Lett.* 542:153-158, 2012.

S. Garashchuk, J. Mazzuca, and T. Vazhappilly. Efficient quantum trajectory representation of wavefunctions evolving in imaginary time. *J. Chem. Phys.* 135:034104, 2011.

RESEARCH FACILITIES

Good research demands excellent facilities and equipment, and the Department of Chemistry and Biochemistry at the University of South Carolina is especially fortunate. In addition to facilities described below and on the following pages, the department maintains an electronics shop and a wide variety of standard and specialized equipment. The department's physical facilities are outfitted with the latest spectrometers as well as instrumentation for kinetics studies, inert atmosphere studies, proteomics, and materials synthesis.

JOHN M. PALMS CENTER FOR GRADUATE SCIENCE RESEARCH

The John M. Palms Center for Graduate Science Research opened in May 2000. The $36 million building totals 158,000 square feet and, except for the basement, is occupied solely by the faculty, staff, and graduate students of the Department of Chemistry and Biochemistry.

The building was designed from the ground up as a chemistry and biochemistry research building and features a state-of-the-art system to control fume hoods and other ventilation apparatus. Sensors determine whether a hood is in use, how high the sash is raised, exhausts, and other information about air quality, which is used by a controller to ensure that flow rates match exacting health and safety standards. The GSRC uses 100 percent outside air; there are no air returns, which also increases safety. To help conserve energy, the hoods alert researchers to lower sashes when leaving their labs at night. The engineered airflow patterns make the building not only much safer but also much more efficient than previous designs.

This leading-edge facility provides space for about 250 scientists. It has 32 faculty offices, 64 four-person labs, 16 two-person labs, and approximately 70 support areas, including instrument space, student and postdoctoral offices, cold rooms, computer areas, and conference rooms. The core facilities of the department—the Mass Spectrometry Center, NMR Center, departmental offices, and stockroom—are located on the first floor for easy access by all researchers.

BIOCHEMICAL INSTRUMENTATION

Sixteen of the research groups in the department are pursuing studies in biochemistry or related areas. A broad range of major instruments supports these investigations. For example, tissue culture facilities are available in several laboratories with sterile hoods, incubators, and microscopes. An Applied Biosystems 380B DNA Synthesizer is used to provide investigators with oligonucleotides (short segments of DNA) of any sequence needed. An Enzyme Kinetics and Thermodynamics Facility features a Hi-Tech SF-61 DX2 double-mixing rapid-scan, stopped flow spectrophotometer equipped with a Hi-Tech MG-6000 diode array detector and a Microcal isothermal titration microcalorimeter. Our Bruker EMXplus EPR spectrometer is equipped with a liquid helium cryostat for studies of metalloproteins at temperatures down to 4 K. An Applied Photophysics SX20 stopped flow spectrophotometer is equipped with a photodiode array, absorption and fluorescence detection to provide sub-millisecond time resolution in photometric studies. The department also has an Agilent model 8453 rapid scanning photodiode array spectrophotometer with Peltier temperature control enzyme kinetic studies. A JASCO model J815 spectropolarimeter is available for circular dichroism measurements. A Biocore 3000 surface plasmon resonance instrument is available for characterization of binding between macromolecules and between macromolecules and small molecules. In addition, we have a share of the Southeast Regional Collaborative Assess Team (SERCAT) that provides twelve 12-hour time slots on the Advanced Photon Source at Argonne National Laboratory.

"I chose to attend USC for my graduate studies because of the high quality faculty, facilities, and research in the department. The collaborative nature of the faculty allows students to perform cutting edge, multidisciplinary research. As a hybrid organic/inorganic chemist, I am working on the development of materials for renewable energy."

—Josef Maier, INORGANIC CHEMISTRY

ELECTRON MICROSCOPY CENTER

The Electron Microscopy Center (EMC), administered by the College of Arts and Sciences, was established in 1970 as the University's central analytical microscopy and imaging facility and has since supported the research activities of more than 2,800 faculty members, graduate students, and undergraduate students. With increased research and educational activities, the EMC has expanded to occupy more than 3,000 square feet in a multi-user, multi-instrument facility on the lower level of the Coker Life Sciences Building. The EMC also assists local industries with service to expand and support product development.

The center provides high resolution microscopy and specimen preparation services for biological and materials science research. In addition, the center offers a graduate level biological microscopy course, necessary training and access to all microscopes and ancillary equipment to faculty, staff, and students of the University of South Carolina System as well as to external users.

The Electron Microscopy Center is operated on a cost-recovery basis and fees are accessed for consumables, equipment use, and staff support. The major shared instruments in the EM Center include a Hitachi H8000 200kV transmission electron microscope (TEM) with digital imaging, a high resolution Zeiss Ultraplus Field Emission Scanning Electron Microscope (SEM) outfitted with an EDAX EDS system, STEM detector, and a Tescan Vega3 SBU variable pressure scanning electron microscope with a back scattered electron detector, Thermo Scientific EDS system and remote operation capability. The ancillary equipment includes a Leica UC7/FC7 cryo-ultramicrotome, room temperature ultramicrotomes, glass knifemaker, vacuum evaporator, sputter coaters, critical point dryer, and light microscopes.

The EMC currently has a full time Research Faculty Director, a master's level staff member and three graduate research assistants with oversight by a faculty committee. A brief description of the major shared equipment is presented below.

- The Zeiss Ultraplus Thermal Field Emission SEM is a high vacuum, high resolution (approximately 1-4 nm) scanning electron microscope with the capability of EDS for elemental analysis. The equipment is outfitted with a charge compensator for non-conductive specimen imaging and a STEM detector. The instrument also has the following detectors: In-lens detector, EsB detector, AsB detector, an Everhart-Thornley secondary electron detector, and a CCD chamberscope with infrared illumination.
- The Hitachi H-8000 TEM has accelerating voltages from 75 to 200 kV. It can provide a magnification from three thousand to five hundred thousand with a resolution of approximately 1nm. The Hitachi TEM is equipped with a side entry goniometer, a SIA L9C bottom mount CCD Camera and is used for soft as well as hard materials imaging.
- The Tescan Vega 3 variable pressure SEM with a resolution of approximately 8-10 nm is equipped with secondary and backscattered electron detectors, an EDS detector for elemental analysis and a chamberscope. This instrument is suitable for both soft and hard materials imaging and can be operated remotely. For further information, please visit the EM Center web page at www.emc.sc.edu.

In a separate facility dedicated to high resolution transmission electron microscopy and operated by the College of Engineering, we have a JEOL JEM 2100F high resolution electron microscope. This instrument is equipped with a field emission gun, a spherical aberration corrector (CEOS), electron energy loss spectroscopy (EELS), energy dispersive x-ray spectroscopy (EDX), tomography and scanning transmission electron microscope (STEM) modes, and high angle annular dark field (HAADF) detector. This instrument is operated by Dr. Douglas Blom, who joined USC in June 2007 from Larry Allard's group at Oakridge National Laboratory.

MAGNETIC RESONANCE FACILITIES

The Nuclear Magnetic Resonance (NMR) Facility consists of four fully multinuclear Fourier transform (FT) NMR Spectrometers. They each have capabilities for advanced single- and multi-dimensional NMR studies.

- **The Varian Mercury/VX 300** is our primary walk-up instrument, and is configured for 1H and 13C observations.
- **The Varian Mercury/VX 400** NMR is a complement to the 300MHz system. Longer time blocks allow users to run more advanced experiments. This system also is used for the bulk of the variable temperature experiments. This system has a 50 sample auto-changer for automated analysis.
- **The Bruker Avance III HD 400 (nanobay)** NMR system features a Prodigy cryo-probe that offers very high sensitivity. A 60 sample auto-changer and auto-tuning capabilities allow for full automation.
- **The Bruker Avance III HD** 500 system's console is equipped with three RF Channels and can perform both liquid and solid-state NMR experiments. 1.9mm and 4mm solid-state MAS probes are available.

The facility's web page at http://homer.chem.sc.edu/nmr contains more details and contact information.

MASS SPECTROMETRY LABORATORY

The Mass Spectrometry Laboratory is located in GSRC room 018 and is equipped with ten mass spectrometers and is open to researchers throughout the University. The instrumentation was funded, in part, by NSF and NIH, as well as a gift from Glaxo-Welcome. A number of additional instruments are located in individual research labs.

- Thermo Orbitrap Velos Pro is a hybrid mass spectrometer consisting of a linear ion trap and an orbitrap mass analyzer. Sample introduction is via a Dionex Ultimate 3000 RSLCnano liquid chromatograph using nanospray ionization. This spectrometer is used for high resolution LC-MS and LC-MS/MS, including data dependent selection of precursor ions. Fragmentation modes include CID, HCD and ETD. This is currently our most sensitive and highest resolution LC-MS instrument and is an excellent instrument for numerous biological/biochemical and trace environmental projects. Experiments include protein detection and identification, location of post translational modifications and differential protein expression analysis.
- Micromass QTOF: Tandem quadrupole-time of flight mass spectrometer for low and high resolution MS and MS/MS by electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI). Sample introduction by direct injection or liquid chromatography. Used primarily for qualitative organic analysis of polar/ionic compounds.
- Micromass QTOF API-USA is a newer version of the QTOF above and is used for special projects that need dedicated set-up time.
- Micromass Quattro-LC: Triple quadrupole mass spectrometer with ESI/APCI. Used primarily for quantitative LC/MS and LC/MS/MS analyses.
- Micromass Quattro-Premier: A newer, more sensitive, version of the Quattro-LC above, this triple quadrupole mass spectrometer is also dedicated to quantitative LC/MS and LC/MS/MS analyses.
- VG 70S: Double-focusing magnetic sector mass spectrometer. Used to obtain EI and CI spectra of compounds introduced by either GC, direct probe, or direct exposure probe. Available fast atom bombardment (FAB) ion source for non-volatile or ionic compounds. Used for high-resolution mass measurement in EI, CI, and FAB modes.
- VG 70S: Identical to the 70S above, this instrument is used primarily for high resolution, quantitative GC/MS.
- Finnigan TSQ: Triple quadrupole instrument dedicated to trace analysis by GC/MS/MS using either electron impact ionization or electron capture negative ionization.
- Bruker Ultraflex MALDI tandem time-of-flight mass spectrometer (TOF/TOF). This instrument allows molecular mass determination of large biomolecules and synthetic polymers using matrix-assisted laser desorption ionization.
- Thermo-Finnigan Element XR ICP-MS: This instrument consists of an inductively coupled argon plasma interfaced to a high resolution magnetic sector mass spectrometer. It is used for trace metals analysis. A restricted access, class 1000, clean room is available for sample preparation.

X-RAY DIFFRACTION FACILITIES

The department maintains a Bruker SMART APEX single crystal diffractometer with a 4K CCD area detector and low-temperature capabilities for small molecule and extended inorganic solid crystal structure determination. The USC NanoCenter, closely affiliated with the department, operates another SMART APEX system. In addition, the following X-ray diffraction instruments are housed in professors' research labs and are available to departmental researchers: a Rigaku R-Axis IV area detector for studies of biological macromolecules, one Rigaku Ultima IV Powder X-ray diffractometer, and one Rigaku D/Max 2100 powder X-ray diffractometer, which has a 1400oC hot stage for variable temperature powder X-ray diffraction studies. The department is also a founding member of the Southeast Region Collaborative Access Team (SER CAT) and has regular access to its X-ray beamlines, which are devoted to biological crystallography. This facility is at the third generation synchroton (Advance Photon Source) located in the Argonne National Laboratory (Chicago area).

FACULTY AND RESEARCH INTERESTS

	ANALYTICAL	BIOANALYTICAL	BIOCHEMISTRY	BIOINORGANIC	BIOORGANIC	BIOPHYSICAL	CATALYSIS	CHEMICAL PHYSICS	CRYSTALLOGRAPHY	ENVIRONMENTAL	FORENSICS	INORGANIC	MATERIALS	MOLECULAR BIOLOGY	NANO	ORGANIC	ORGANOMETALLIC	PHYSICAL	POLYMER	SOLID STATE	SPECTROSCOPY	SUPRAMOLECULAR	THEORETICAL/ COMPUTATIONAL
ADAMS							■		■			■	■		■		■						
ANGEL	■									■			■		■			■			■		
BENICEWICZ													■		■	■			■				
BERG						■		■					■		■			■	■		■		■
CHEN	■						■	■				■	■		■			■		■	■		
CHRUSZCZ			■			■	■		■					■									
DAWSON			■	■	■	■	■					■									■		
FERRY	■	■					■			■					■			■			■		
GARASHCHUK								■							■			■					■
GOODE	■										■	■									■		
GREYTAK									■			■	■		■			■		■	■	■	
KARTHIKEYAN			■											■									
LAVIGNE	■		■		■								■		■	■	■		■			■	
MAKRIS			■	■	■	■	■		■			■		■							■		
MORGAN	■	■								■	■								■		■		■
MYRICK	■									■	■		■					■			■		■
C. E. OUTTEN			■	■		■								■									
F. W. OUTTEN			■	■						■		■		■									
PERYSHKOV							■						■				■						
RASSOLOV								■							■			■					■
REGER									■			■				■	■					■	
RICHARDSON	■									■		■				■		■			■		
SHAW	■									■		■									■		
K. SHIMIZU													■		■	■		■	■			■	
L. SHIMIZU			■		■		■		■				■		■	■				■	■	■	
SHUSTOVA							■		■			■	■			■		■		■		■	
STEFIK							■		■			■	■		■	■			■	■		■	
SODETZ			■						■					■									
TANG													■		■	■	■		■			■	
VANNUCCI							■					■	■				■						
VOGT							■	■	■	■		■	■		■			■		■			■
H. WANG						■							■	■	■			■			■		
Q. WANG					■								■		■	■			■			■	
WISKUR							■									■	■					■	
ZUR LOYE									■			■	■		■					■		■	

RICHARD D. ADAMS

CAROLINA DISTINGUISHED PROFESSOR

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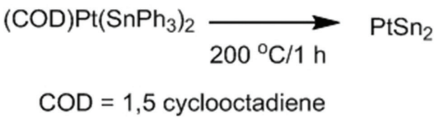
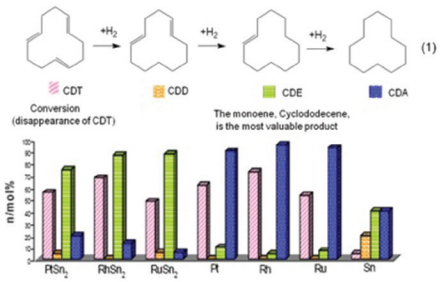
B.S., 1969, Pennsylvania State University; Ph.D., 1973, Massachusetts Institute of Technology.

Alfred P. Sloan Foundation Research Fellow, 1979–83; Russell Research Award for Science, Mathematics, and Engineering, University of South Carolina, 1989; regional editor, Journal of Organometallic Chemistry; co-editor, Journal of Cluster Science; Charles Holmes Herty Medal, ACS Georgia Section, 1999; Charles H. Stone Award, ACS Carolina Piedmont Section, 1999; Chemical Pioneer Award, American Institute of Chemists, 2000; Senior Scientist Award, Alexander von Humboldt Foundation, 2000; Outstanding South Carolina Chemist, ACS South Carolina Section, 2001; Southern Chemist Award, ACS Memphis Section, 2001; South Carolina Governor's Award for Excellence in Science, 2003; Fellow of the American Association for the Advancement of Science, 2003; Carolina Trustee Professor, 2005; Henry J. Albert Award of the International Precious Metals Institute, 2005. American Chemical Society Award for Distinguished Service in the Advancement of Inorganic Chemistry, 2010; Southeastern Universities Research Association Distinguished Scientist Award, 2011; Member of the European Academy of Sciences and Arts, 2011.

Research Areas: Bimetallic Complexes for Applications in Catalysis; Studies of the synthesis, structures, and catalytic properties of unsaturated bimetallic clusters and nanoparticles for hydrogen activation and selective oxidation reactions.

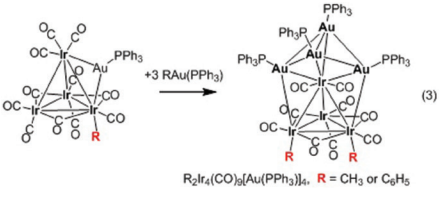
Research: The chemical industry relies on the use of reaction catalysts derived from the elements of the transition series for the economical production of many of the great variety of petro- and commodity chemicals in use today. Studies have shown that bi- and multimetallic catalysts often exhibit properties that are superior to those of the individual metal components. Synergism and bifunctional activity are two of the ways that this superior performance is achieved. It has been found that the addition of metals from main groups of elements, such as tin, can also significantly improve the activity and selectivity of transition metal (TM) catalysts still further. Our research has been focused on synthesizing bi- and multimetallic complexes for use a precursors to new stiochiometrically-precise multimetallic nanoparticles on supports for use as reaction catalysts. For example, we have recently shown that transition metal cluster complexes containing tin ligands are precursors to superior heterogeneous nanocatalysts that selectively hydrogenate 1, 5, 9-cyclododecatrene CDT to cyclododecene CDE. CDE is an important

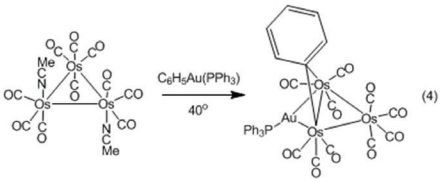




chemical feedstock for the production of polymers such as nylon-12.

Nano-gold has recently been found to be a valuable catalyst for selective oxidation catalysis. It has already been shown that high activity oxidation catalysts can be obtained by mixing gold with the more traditional transition metal catalysts. To expand upon work in this area, we have been synthesizing new bimetallic transition metal – gold complexes for the purpose if creating new bimetallic TM-Au catalysts for selective oxidation reactions. For example, we have prepared new iridium-gold and osmium-gold complexes by reactions of the organogold complexes $(Ph_3P)AuR$, R = CH_3 and





C_6H_5 with activated forms of iridium carbonyl and osmium carbonyl, see eqs. (3) and (4).

Representative Publications

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Adams, R. D.; M. Chen, Xinzheng Yang, Iridium-Gold Cluster Compounds. Syntheses, Structures and an Unusual Ligand-Induced Skeletal Rearrangement. *Organometallics* **2012**, 31, 3588–3598.

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Adams, R. D.; Captain, B. Hydrogen Activation by Unsaturated Mixed Metal Cluster Complexes: New Directions, *Angew. Chem. Int. Ed.* **2008**, 47, 252-257.

S.MICHAEL ANGEL

PROFESSOR; FRED M. WEISSMAN CHAIR IN CHEMICAL ECOLOGY

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In LIBS, the sample is ablated and ionized using a pulsed laser. Analysis of the emission from the plasma provides information on the elemental composition of the sample. This technique is unique in that elemental composition can be determined remotely.

B.S., 1979, North Carolina State University; Ph.D., 1984, North Carolina State University; Postdoctoral Fellow, 1985–1986, Lawrence Livermore National Laboratory.

Physics and Advanced Technologies Directorate Award, 2006; Georgia Southern State University, student seminar program featured research, 2006; Editorial Board Member of International Journal of Spectroscopy; A-Page Advisory Panel Member for Analytical Chemistry; Advisory board of TALANTA; International Scientific Committee Member NASLIBS, 2007;Tour Speaker for Society of Applied Spectroscopy (SAS), 2007; USC Educational Foundation Research Award for Science, Mathematics and Engineering, 2009; Elected Fellow AAAS, 2011; FACSS Innovation Award, 2011; Mortar Board Excellence in Teaching award, 2011; SCIX Innovation Award Winner 2011; SC Section ACS Outstanding Chemist Award, 2012; SAS Meggers Award, 2012; Carolina Trustee Professorship award, 2013; Invited Tour Speaker for the Society for Applied Spectroscopy, 2014.

Research Areas: Development of *in-situ* characterization techniques including fiber-optic chemical sensors and remote spectroscopy including Raman, LIBS and REMPI. Of particular interest is applying optical spectroscopy to remote measurements in extreme environments and development of fieldable spectroscopic instrumentation.

We are exploring a number of remote spectroscopic techniques and sensors for noncontact and *in-situ* measurements. Such techniques allow unique applications in environmental, marine, earth, and space science. For example in past research, microimaging sensors were used for in situ measurements of analyte diffusion in thin membranes and in other work resonance enhanced multiphoton laser ionization, REMPI, was used to measure ppb levels of toxic compounds in soil samples. In more recent work, laser-induced breakdown spectroscopy, LIBS, is used for remote, noncontact elemental analysis and is being applied to *in-situ* chemical measurements in the deep ocean (see figure at above). Other techniques being explored include standoff Raman spectroscopy and Raman imaging for planetary and homeland security applications.

Fiber-optics are used for many *in-situ* measurements. In this case, light transmitted to the sample region via the fiber optic is used to perform a direct spectroscopic measurement. This type of analysis is referred to as remote fiber spectroscopy (RFS) and encompasses many spectroscopic methods, such as Raman, surface-enhanced Raman, absorption, reflectance, LIBS, REMPI, and fluorescence spectroscopies that have been adapted for use with optical fibers. We are also interested in the use of optical fibers as chemical sensors where the transmitted light probes an intermediate material affixed to the terminal end of the fiber that interacts with a target molecule to produce an optical signal.

Recently our focus has been on deep-ocean applications of LIBS, and standoff Raman spectroscopy for measuring hazardous materials and for planetary applications. LIBS is difficult in bulk aqueous solution because the laser-induced plasma is rapidly quenched by water. The quenching problem can be overcome by using laser pulse pairs, where a water bubble created by the first laser pulse isolates the LIBS plasma that is formed by the second laser pulse and trapped in the bubble. It is hoped that this technique will allow LIBS to be used for elemental analysis of hydrothermal vent fluids at 2–3 km depths. Homeland defense applications of standoff Raman spectroscopy include detection of high explosive materials at many 10s of meters distance. Our recent investigations of standoff Raman spectroscopy for planetary applications has led to the development of a new type of Fourier transform Raman spectrometer, the spatial heterodyne Raman spectrometer, that could lead to much smaller and more rugged Raman instruments suitable for planetary lander missions. This work also led to the first published description of an orbital Raman spectrometer suitable for surface Raman measurements.

Representative Publications

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Register, J.; Scaffidi, J.; Angel, S. M. Direct Measurements of Sample Heating by a Laser-induced Air Plasma in Pre-Ablation Spark Dual-Pulse Laser-Induced Breakdown Spectroscopy (LIBS). *Appl. Spectrosc.* **2012**, 66, 869-874.

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Pearman, W. F.; Carter, J. C.; Angel, S. M.; Chan, J. W-J. Quantitative measurements of CO_2 and CH_4 using a multipass Raman capillary cell. *Appl. Opt.* **2008**, 47, 4627-4632.

Pearman, W. F.; Michael, S. A.; Ferry, J. F.; Sherwood, H. Characterization of the Ag Mediated Surface-Enhanced Raman Spectroscopy of Saxitoxin. *Appl. Spectrosc.* **2008**, 62, 727-732.

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BRIAN C. BENICEWICZ

EDUCATIONAL FOUNDATION DISTINGUISHED PROFESSOR; COEE CHAIR IN POLYMER NANOCOMPOSITE RESEARCH

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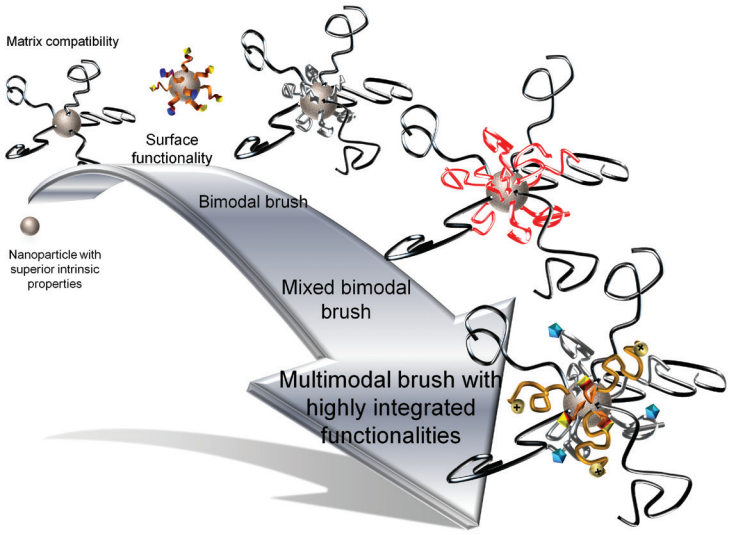

B.S. 1976, Florida Institute of Technology; Ph.D., 1980, University of Connecticut; Research Scientist, 1980–1982, Celanese Research Co.; Senior Scientist, 1982–1985, Ethicon, Inc.; Staff Member, Section Leader, Deputy Group Leader, Los Alamos National Laboratory, 1985–1997; Professor and Director of the Center for Polymer Synthesis, Rensselaer Polytechnic Institute, 1997–2008.

Los Alamos National Laboratory "Excellence in Industrial Partnership Award", 1996; Los Alamos National Laboratory Distinguished Patent Award, 1997; NASA Technology Achievement Award, 1997; NASA Technology Program Award, 1998; Chair, Gordon Conference on Fuel Cells, 2006; Fellow, AAAS, 2011.

Research Areas: Polymer-organic chemistry, new monomer and polymer synthesis, polymer nanocomposites, polymer membranes for fuel cells, electrically conducting polymers, liquid crystalline polymers, controlled radical polymerization.

The underlying theme for all of the work in our group is our ability to synthesize polymers by new methods and with properties or combinations of properties not found in existing materials. We simply enjoy making new materials. However, our work extends beyond the synthesis, and we characterize the properties of these new materials and test them in potential applications to establish structure-property relationships to further aid in the design of next generation polymers.

Polymer Nanocomposites: We are developing controlled radical polymerization techniques to design the interfacial properties of polymer nanocomposites. We have developed a toolbox of methods to control the chemistry at the surface of nanoparticles with great precision and use "click" chemistry techniques to introduce functionalities at the surface of nanoparticles which could not survive the polymerization conditions or may interfere with the polymerization. Block copolymerization is also used to establish multilayers at the nanoparticle surface. Our work relies on the use of the controlled radical polymerization technique, RAFT, or reversible addition-fragmentation, chain transfer polymerization. The design of new RAFT agents, surface anchored RAFT agents, and new monomers have allowed us to prepare surface functionalized nanoparticles for many different applications.

Fuel Cell Membranes: We are investigating new polymers for high temperature fuel cell membranes. The polymer membrane is considered the "heart" of a polymer electrolyte membrane (PEM) fuel cell and represents a central challenge for the future of fuel cell devices. Polybenzimidazoles imbibed with phosphoric acid are being prepared and tested in fuel cells at temperatures up to 200˚C. Our work over the last several years has been focused on a new process that allows high phosphoric acid levels while still maintaining the mechanical strength for these highly loaded films. The conductivities and fuel cell performance have increased substantially and now exhibit values suitable for commercial applications.

We have also explored a great deal of new chemistry associated with the basic synthetic methods and new compositions to further improve the basic conductivity of the polymer membrane. The synthesis of new compositions continues with the belief that the polymer plays an important role in the conductivity. An extensive fuel cell test laboratory designed for high temperature membrane testing supports our work in this area. We have also extended this work to investigate electrochemical hydrogen pumping for hydrogen separation and purification applications.

REPRESENTATIVE PUBLICATIONS

Li, Y.; Krentz, T.; Wang, L.; Benicewicz, B.C.; Schadler, L.S. Ligand Engineering of Polymer Nanocomposites: From the Simple to the Complex. *ACS Appl. Mat. & Interfaces.* **2014**, asap.

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Moll, J.; Kumar, S.K.; Snijkers, F.; Vlassopoulos, D.; Rungta, A.; Benicewicz, B.; Gomez, E.; Ilavsky, J.; Colby, R. Dispersing Grafted Nanoparticle Assemblies into Polymer Melts through Flow Fields. *ACS Macro Lett.* **2013**, 2, 1051-1055.

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Li, J.; Benicewicz, B.C. Synthesis of Well-Defined Side-Chain Fullerene Polymers and Study of their Self-Aggregation Behaviors. *J. Polym. Sci., Polym. Chem.* **2013**, 51, 3572-3582.

MARK A. BERG

PROFESSOR

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B.S., 1979, University of Minnesota; Ph.D., 1985, University of California at Berkeley; Postdoctoral Fellow, 1985–1987, Stanford University.

Camille and Henry Dreyfus Distinguished Young Faculty Award, 1987; National Science Foundation Presidential Young Investigator, 1990; Alfred P. Sloan Foundation Research Fellow, 1992; Fellow of the American Physical Society, 2000; USC Educational Foundation Research Award, 2007; SC Section ACS Outstanding Chemist Award, 2014.

Research Areas: Ultrafast laser spectroscopy; dynamics of molecules in liquids, glasses, polymers and other complex materials; development of new multiple-pulse spectroscopies.

Just as the static properties of macroscopic materials are determined by structure on Angstrom to nanometer length scales, the macroscopic, dynamic properties are determined by motion on the femtosecond to nanosecond time scales. For example, single-collision times in solids and liquids are near 0.1 ps; sound waves transmit conformational changes across a 10 nm diameter protein in 10 ps; solar energy captured by a semiconductor nanoparticle persists no longer than a few 10's of ns. If we want to understand the macroscopic behavior of materials in terms of molecular properties, experiments on these ultrafast time scales are required.

Although these times are natural for molecular processes, they can only be measured by using ultrafast laser technology. In our laboratory, pulses with durations as short as 50 fs and with peak intensities in the 10 Gigawatt range are used to investigate these processes. These pulses are only 15 microns in physical length. They consist of 15–20 optical cycles if they are in the visible and only a few cycles if they are in the infrared. Using these pulses, we observe events as fast as the breaking of a chemical bond or of a single collision in solution.

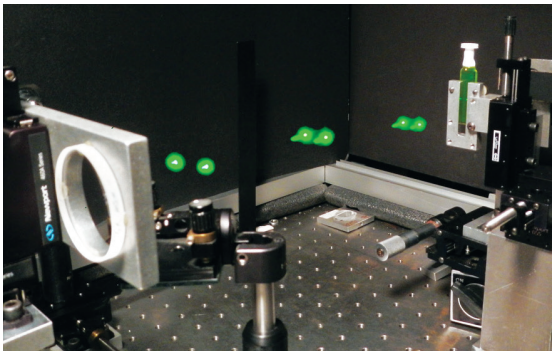

Fig. 1. New methods using the coordinated action of six, ultrafast laser pulses can separate the dynamics of different molecular subensembles within a heterogeneous sample. The pulses (green) have passed through the lens on the left and are being focusing onto a common point in the sample (green cuvette) on the right.

In addition to ultrafast lasers, our experiments need new methods to measure molecular motion using only pulses of light. We are actively developing complex sequences of pulses to measure new properties. These "multidimensional" spectroscopies exploit both the high intensity electric fields in the laser pulses and the fact that materials retain memory of the phase of their excitation during these short times. We have recently demonstrated that a sequence of six pulses (called a MUPPETS experiment) can measure the electronic-relaxation rate of specific subpopulations within a heterogeneous sample. A number of other new, but related, measurements have been predicted and are being brought into the laboratory to address problems of current interest. Examples include:

Energy Pathways in Nanostructures. Semiconducting nanostructures offer great promise for harvesting solar energy, but no two nanostructures are ever identical at the atomic level. Lattice defects, variation in surface structure and misplaced passivating molecules are common and can greatly affect energy flow, but are difficult to detect in structural measurements. MUPPETS offers a means to measure the different fates of energy in different particles within a real sample.

Peptide Dynamics. In some circumstances, proteins do not have a well defined structure: before folding, after denaturation, in "intrinsically disordered" proteins, and in short peptides. The speed of conformational changes makes it difficult to characterize either the range of conformations or the rate of interconversion between them. Ultrafast multidimensional experiments coupled with FRET (fluorescence resonance energy transfer) is a new approach that will be used to make these measurements.

Glass Dynamics. At temperatures very near the glass transition, there is strong evidence that the liquid breaks up into microscopic regions of differing viscosity. Polarization-resolved MUPPETS measurements offer a route to trace this heterogeneity to its origins at higher temperatures and shorter relaxation times.

Our research draws on chemistry, laser physics, statistical mechanics, spectroscopy, and biology to answer broad issues in chemistry, physics, and materials science. Students with a background in any of these field can contribute to our efforts. Growth into unfamiliar areas is expected and is facilitated by interactions with students and postdocs from a variety of fields.

Representative Publications

Wu, H.; Berg, M. A. Multiple Populations-Period Transient Spectroscopy (MUPPETS) in Excitonic Systems. *J. Chem. Phys.* **2013**,138, 034201.

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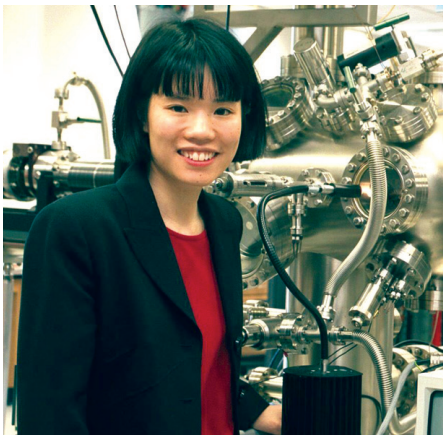

DONNA A. CHEN

PROFESSOR; ADJUNCT PROFESSOR IN CHEMICAL ENGINEERING

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B.S., 1992, Rochester Institute of Technology; Ph.D., 1997, Harvard University; Postdoctoral Fellow 1997–1999, Sandia National Laboratories.

Army Young Investigator Award, 2000; NSF CAREER Award, 2002; South Carolina Governor's Young Researcher Award for Excellence in Science, 2008; Michael J. Mungo Undergraduate Teaching Award, 2010; Finalist for Ada B. Thomas Outstanding Faculty Advisor Award, 2011-2013; International Precious Metals Carol Tyler Award, 2013.

Research Areas: Reactions at surfaces, reaction mechanisms, scanning probe microscopy, characterization of surfaces, chemistry of metal nanoparticles, catalysis.

Research in the Chen group focuses on understanding surface chemistry on the atomic and molecular level. One of the main motivations of this work is to gain a fundamental understanding of atomic processes on surfaces in order to guide the development of new materials for heterogeneous catalysts. Most commercial catalysts consist of metal particles on an oxide support, and it is therefore important to have a fundamental understanding of the reaction processes occurring on the surfaces of the metal particles in order to systematically design catalytic materials with activity and selectivity that can be tailored for specific chemical reactions.

Since the commercial catalysts are complex materials, we are studying model systems consisting of metal particles supported on single-crystal surfaces. Specifically, we are growing metal nanoparticles on oxide surfaces and studying the chemical activity of these nanoparticles as a function of their size, structure, interactions with the oxide support, and metal-metal interactions in bimetallic particles. In these model systems, metal particles are vapor-deposited onto single-crystal oxide surfaces with controlled sizes and size distributions. As an example, Figure 1a below shows scanning tunneling microscopy (STM) images of Au particles on a rutile TiO_2(110), Figure 1b shows Ni-Au bimetallic particles on TiO_2 at room temperature (~1.2 nm high), and Figure 1c shows the Ni-Au particles after heating the surface to 800 K (~1.4 nm high). Quantum effects, unique surface structures for the nanoparticles, and interactions between the particles and support are all size-dependent phenomena that can give rise to enhanced or modified activity for catalysts when their particle sizes are controlled in the nanoscale range.

Recently, we have been studying oxidation reactions on bimetallic Au-based nanoparticles (Au-Pt, Au-Ni, Au-Co) on titania; despite the inactivity of bulk Au surfaces, Au/TiO_2 is a good catalysts for the low temperature oxidation of CO to CO_2 and propylene to propylene oxide. In these systems, interactions between the two metals and between the metal and titania support are known to give rise to unusual chemistry. For example, new surface sites are created at the edges of Au particles on titania, and these sites at the perimeter of the particles are active for the oxidation of methanol to formaldehyde. Exposing the bimetallic particles to reactant gases results in changes in the surface composition, which determines the chemical activity of the clusters. In other bimetallic systems, such as Pt-Re and Pt-Co, electronic interactions between the metals are used to alter chemical activity. We have developed a protocol for growing exclusively bimetallic clusters by taking advantage of the different diffusion rates for the metals on the surface and selectively nucleating the more mobile metal at seed clusters of the less mobile metal. Futhermore, Pt-Ru bimetallic catalysts for direct methanol fuel cells have been grown in solution on the single-crystal supports using electroles deposition methods in conjunction with our collaborators in the Chemical Engineering Department; the properties of these catalyst are compared with those prepared by vapor-deposition.

Most of our experiments are carried out in ultrahigh vacuum (UHV) chambers with pressures of $<1x10^{-10}$ Torr. This provides us with a well-controlled environment in which we can control the composition of the surface on the atomic level. STM is used to characterize sizes and shapes of deposited metal nanoparticles on the atomic scale. X-ray photoelectron spectroscopy (XPS), low energy ion scattering (LEIS), low energy electron diffraction (LEED), temperature programmed desorption (TPD, a form of mass spectrometry) and other surface analysis techniques provide information on surface structure, atomic composition, chemical bonding, and identification of reaction products. A prototype catalytic reactor coupled to the UHV system allows us to evaluate reaction kinetics on the model surfaces under realistic catalytic conditions. We are also currently constructing an infrared spectroscopy system (polarization modulation infrared absorption reflection spectroscopy) capable of studying the surfaces during catalytic reactions at elevated pressures. Ambient-pressure XPS experiments are conducted at the National Synchrotron Light Source at Brookhaven National Laboratory

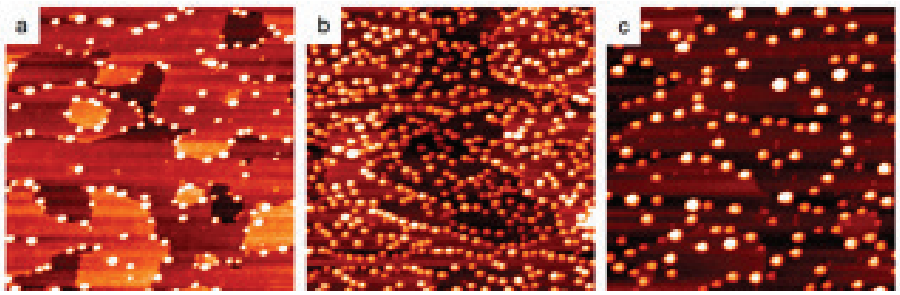

Figure 1: STM images of Au and Au-Ni nanoparticles on TiO_2. See text for more details. All images are 100x100nm^2

Representative Publications

Tenney, S. A.; Shah, S. I.; Yan, H.; Cagg, B. A.; Levine, M. S.; Rahman, T. S.; Chen, D. A. Methanol Reaction on Pt-Au Clusters on TiO_2(110): Methoxy-induced Diffusion of Pt. *J. Phys. Chem. C* **2013**, 117, 26998-27006.

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Galhenage, R. P.; Yan, H.; Tenney, S. A.; Park, N.; Henkelman, G.; Albrecht, P.; Mullins, D. R.; Chen, D. A. Understanding the Nucleation and Growth of Metals on TiO_2: Co Compared to Au, Ni and Pt. *J. Phys. Chem. C* **2013**, 117, 7191.

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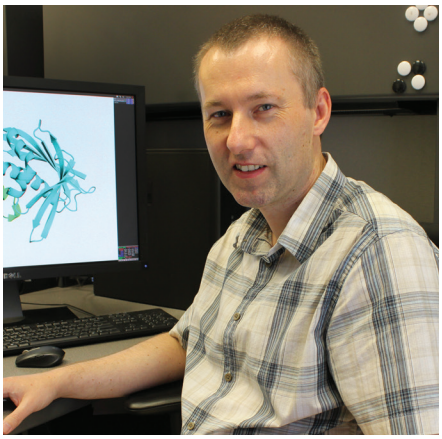
Tenney, S. A.; He, W.; Ratliff, J. S.; Mullins, D. R.; Chen, D. A. Characterization of Pt-Au and Ni-Au Clusters on TiO_2(110). *Top. Catalysis* **2011**, 54, 42.

Tenney, S. A.; Ratliff, J. S.; He, W.; Roberts, C. C.; Ammal, S. C.; Heyden, A.; Chen, D. A. Adsorbate-Induced Changes in the Surface Composition of Bimetallic Clusters: Au-Pt on TiO_2(110). *J. Phys. Chem. C* **2010**, 114, 21652.



MAKSYMILIAN CHRUSZCZ

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Research Areas: Structural Biology, Allergy & Asthma, Host-Pathogen Interactions, Immunology

My group studies the interactions of the human immune system with pathogens and allergens. We are interested in the ways by which pathogens and allergens deregulate or deceive the immune system, and how such processes influence human health. In addition, our research interests include mechanisms of bacterial growth in mammalian host organisms, with a special emphasis on a microorganism's ability to acquire nutrients from the host. We are using multiple experimental and computational techniques in a "from atoms to animals/humans" approach, which correlates *in vitro* functional and structural analyses of macromolecules with studies of in vivo systems, like cells and model organisms.

Currently there are approximately 1100 officially registered allergens, with less than 10% having an experimentally determined three-dimensional structure. We believe that large scale structural studies are indispensable for significantly improving our knowledge of allergens and their impact on human health. Thus, we use a variety of structural biology techniques (including X-ray crystallography and others) to obtain experimental models of proteins of interest.

Food allergens. Current knowledge of food allergens is limited. For example, it is not known why some plants proteins are very potent allergens (like peanut or tree nut allergens), while similar proteins from closely related plants do not pose a significant allergenic risk. In order to address this question we analyze several groups of plant proteins important both to agriculture and human health.

One such group of proteins comprises peanut allergens (Figure 1). Peanut allergens alone affect 1% of the population in the US and often cause anaphylaxis, the most dangerous—and potentially life-threatening—manifestation of allergic diseases. We are working both on recombinant allergens and those isolated from natural sources. Studies of natural allergens are especially important, because in many cases it is difficult to demonstrate the same IgE binding properties in recombinant proteins as seen in natural allergens. Differences in IgE binding properties between recombinant and natural versions of allergens may indicate that in diagnostic tests the recombinant protein is not a suitable replacement for the allergen derived from its natural source.

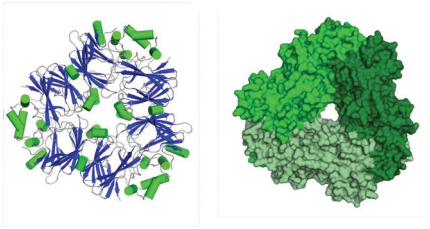

Figure 1. The trimeric form of the Ara h 1 core fragment represented in cartoon representation (left) and as a molecular surface (right). The four major peanut allergens are Ara h 1, a vicilin protein, Ara h 3, a legumin, and two 2S albumins (Ara h 2 and Ara h 6).

Inhaled allergens. Our group is also working on several inhaled allergens. For example, we are studying Group 1 dust mite allergens (Der f 1 and Der p 1), which are believed to be among the most potent triggers of asthma. Most mite allergic patients (>80%) have IgE antibodies against the Group 1 mite allergens, Der f 1 and Der p 1. These allergens are cysteine proteases (Figure 2) and their proteolytic activity contributes significantly to allergenicity. Der p 1 cleaves the CD23 and CD25 receptors, and the cleavage of these receptors favors a Th2 response and induction of release of pro-inflammatory cytokines from bronchial epithelial cells, mast cells and basophils. The resulting increase in IgE antibody synthesis and inflammation of lung epithelium may explain why mite allergens are strongly associated with asthma.

Bacterial proteins. Our group is also working on several bacterial proteins originating from *Streptococcus pyogenes, Vibrio vulnificus* and *Wolbachia* species. We are interested in proteins involved in production of toxins, as well as in proteins which are

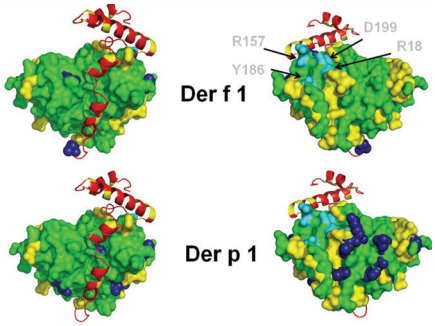

Figure 2. The molecular surface of Der f 1. Residues that differ in Der f 1 and Der p 1 are shown in yellow. Amino acids substitutions in different polymorphic variants of Der p 1 and Der f 1 are presented in dark blue. Residues binding a cross-reactive monoclonal antibody are shown in blue. The N-terminal pro-peptide is shown in ribbon representation (red).

targets for potential antimicrobial compounds. For example, we study dihydropicolinate reductase and 1-deoxy-D-xylulose-5-phosphate reductoisomerase from V. *vulnificus.* Both proteins are potential drug targets as they are critical parts of bacterial metabolic pathways, which are not present in humans. Dihydropicolinate reductase is a part of the pathway leading to lysine and peptidoglycan synthesis, while 1-deoxy-D-xylulose-5-phosphate reductoisomerase is involved in steroid synthesis in the non-mevalonate pathway.

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Offermann, L. R.; Chan, S. L.; Osinski, T.; Tan, Y. W.; Chew, F. T.; Sivaraman, J.; Mok, Y-K.; Minor, W.; Chruszcz, M. The major cockroach allergen Bla g 4 binds tyramine and octopamine. *Mol. Immunol.* **2014**, 60, 86-94.

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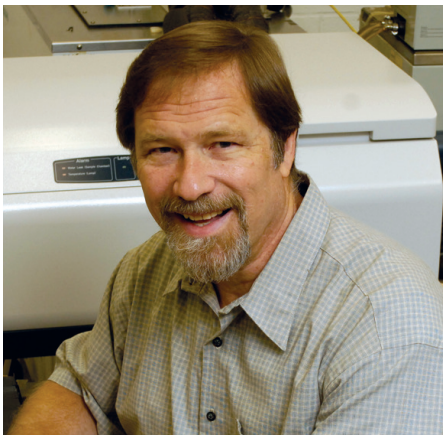

JOHN H. DAWSON

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A.B., 1972, Columbia University; Ph.D., 1976, Stanford University; NIH Postdoctoral Fellow, 1976–1978, California Institute of Technology.

Camille and Henry Dreyfus Teacher-Scholar, 1982-87; Alfred P. Sloan Research Fellow, 1983-1987; NIH Research Career Development Award, 1983-1988; Outstanding South Carolina Chemist, SC Section, American Chemical Society, 1988; Russell Research Award for Science, University of South Carolina, 1988; Elected Fellow, American Association for the Advancement of Science, 1989; Editorial Board, Chemtracts-Inorganic Chemistry, 1992-present; Basic Science Research Award, University of South Carolina School of Medicine, 1993; Editor-in-Chief, Journal of Inorganic Biochemistry, 1996-present; Governor's Award for Excellence in Science, 1997; Conference Chair, Tenth International Conference on Cytochrome P-450, 1997; Chair, Bioinorganic Subdivision, Inorganic Division, American Chemical Society, 2000; Editorial Board, Journal of Biological Chemistry, 2002-2007; Southern Chemist Award, Memphis Section, American Chemical Society, 2003; Carolina Trustee Professor Award, University of South Carolina, 2004; Chair, Metal Ions in Biology Gordon Research Conference, 2005; Charles H. Stone Award, Charlotte/Piedmont Section, American Chemical Society, 2006; Wyeth/Alumni Lecture, Columbia University, 2006; Elected Fellow, American Chemical Society, 2010; University of South Carolina Educational Foundation Outstanding Service Award, 2012.

Research Areas: Bio-inorganic, bio-physical, and bio-organic chemistry; spectroscopy and mechanisms of action of dioxygen- and peroxide-activating heme iron enzymes and model systems; cytochrome P-450; magnetic circular dichroism spectroscopy.

The mechanism of dioxygen activation for insertion into organic molecules is a problem of fundamental importance. The enzymes that catalyze these transformations often require metal ions for activity. Results obtained from the investigation of such metallo-enzymes, in addition to providing insight into their mechanism of action, are of obvious relevance to the design of catalysts for non-enzymatic oxidations. My research interests focus on the structure and function of dioxygen- and peroxide-activating heme iron enzymes. Additional areas of interest include the role of metal ions in enzymatic catalysis and structure, structural and functional model systems, and the application of magnetic circular dichroism, X-ray absorption, and electron paramagnetic resonance spectroscopy to bioinorganic systems.

Two experimental approaches are being used: (a) spectroscopic studies to establish the structure of the metal binding site and (b) mechanistic investigations to define the molecular sequence of events involved in catalysis. All appropriate spectroscopic methods are being used to accomplish the first of these two goals. The mechanistic studies involve the use of cryoenzymology and rapid kinetic techniques such as stopped-flow rapid-scanning absorption spectroscopy and freeze-quenching, as well as the determination of important mechanistic parameters.

Cytochrome P-450 has been the focus of research in my lab for many years. This heme enzyme has unusual spectroscopic properties and catalytic reactivities relative to other heme enzymes. Its ability to oxygenate an extensive range of substrates has generated considerable interest in its mode of action. In addition to spectroscopically examining the accessible stable states of this enzyme, emphasis is being placed on a detailed understanding of the substrate and ligand binding processes and on attempts to trap out the reactive intermediates responsible for oxygen insertion.

In collaboration with Professor Lukasz Lebioda, we are studying two fascinating heme-containing peroxidases from marine sources. One halogenates aromatic substrates (phenols) and the other dehalogenates the resulting halophenol products. Both have unusual spectroscopic and mechanistic properties, relative to other peroxidases, that challenge the conventional structure-function patterns of heme-containing peroxidases.

Magnetic circular dichroism (MCD) spectroscopy is a particularly powerful technique for studying heme systems because of its frequent ability to distinguish between porphyrin structures with different axial ligands. To expand the utility of this technique, we are studying the spectroscopic properties of porphyrin complexes of known structure and numerous heme proteins such as nitric oxide synthase, allene oxide synthase and a variety of heme binding and transport proteins. We have both UV-visible and near-IR MCD spectrophotometers, the latter for studying low-energy structure-sensitive charge transfer transitions.

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JOHN L. FERRY

PROFESSOR

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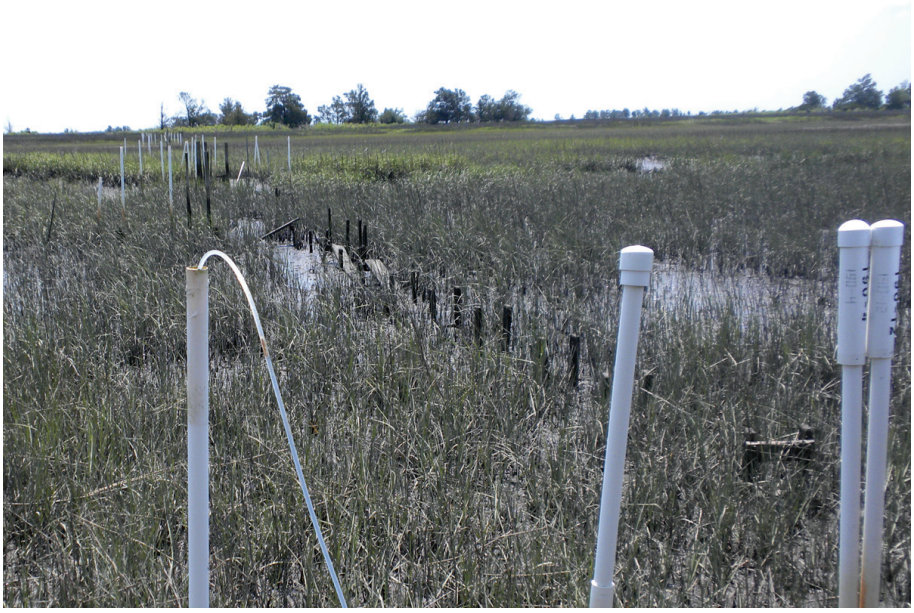
B.S., 1990, University of Illinois-Urbana; M.S., 1993, University of North Carolina; Ph.D., 1996, University of North Carolina-Chapel Hill; Postdoctoral Fellow, 1996–1998 University of Texas-Austin.

Michael J. Mungo Award for Undergraduate Teaching, 2012



Research Areas: Environmental chemistry; fate and transport of organic chemicals in the environment; water chemistry; photochemically driven oxidation; photocatalysis; trace organic analysis; combinatorial chemistry; free radical chemistry.

Introduction: My research is broadly centered on studying the fate of organic chemicals in the environment. This includes man-made chemicals like pollutants, pharmaceuticals and pesticides; and also naturally occurring chemicals like biotoxins, signaling molecules and various plant products. My group applies advanced analytical techniques to learn how these chemicals are transformed in or removed from the environment.

Analytical approaches: Environmental analyses need to be fast, sensitive and selective. We use whatever analytical tools we need to, but most often work with gas or liquid chromatographs with mass spectrometric or spectroscopic detectors. We also use absorbance or fluorescence spectroscopy (steady state and time resolved); various electrochemical techniques, nuclear magnetic resonance spectroscopy, infrared spectroscopy, and transmission electron microscopy.

Experimental approaches: Environmental chemists spend time in the field making measurements and in the laboratory testing explanations for their field work. My group has done field work measuring the fate and distribution of organic chemicals, nanoparticles, transition metals, and oxidants like hydrogen peroxide or the hydroxyl radical. We quantify the relationships between those analytes in the laboratory with sophisticated environmental modeling techniques. We use robotic systems to generate solutions modeling hundreds of different environmental conditions simultaneously, a process called combinatorial environmental chemistry. These solutions are spiked with a variety of probe molecules and contaminants, and then subjected to weathering processes in the laboratory. This allows us to rapidly interrogate environmental systems for their ability to promote photodegradation, free radical oxidation, complexation of transition metals, etc. Coupling this approach with field monitoring is one of the surest ways to make sound predictions about what will happen to pollutants as they are processed by environmental systems.

Representative Publications

Murphy, S. A.; Solomon, B. M.; Meng, S. N.; Copeland, J. M.; Shaw, T. J.; Ferry, J. L. Geochemical Production of Reactive Oxygen Species From Biogeochemically Reduced Fe. *Environ. Sci. Technol.* **2014**, 48(7), 3815-3821.

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Decho, A. W.; Visscher, P. T.; Ferry, J. L.; Kawaguchi, T.; He, L.; Przekop, K. M.; Norman, S. R.; Reid, P. R. Autoinducers extracted from microbial mats reveal a surprising diversity of N-acylhomoserine lactones (AHL) and abundance changes that may relate to diel pH. *Environ. Microbiol.* **2009**, 11(2), 409-420.

SOPHYA GARASHCHUK

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M.S., Physics, 1992, Moscow Institute of Physics and Technology, Ph.D., 1999, University of Notre Dame Postdoctoral Fellow, 1999–2001, University of Chicago.

IBM-Lowdin Fellowship, 2004; Sanibel symposium; Doctoral New Investigator ACS-PRF, 2011; NSF CAREER Award, 2011; USC Breakthrough Rising Star, 2012.

Research Areas: Theoretical and computational chemistry including quantum effects in dynamics of nuclei, development of approximate quantum potential method applicable to large molecular systems and studies and quantum tunneling during proton transfer processes.

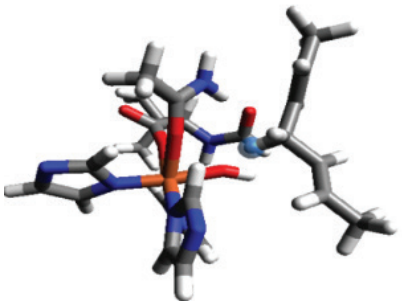

Fig 1: Proton transfer in soybean lypoxygenase-1. Quantum nature of nuclear motion can be crucial for reactions in condensed phase. For example, proton transfer in SLO-1 proceeds by tunneling. We use quantum trajectory dynamics developed in the group, to incorporate quantum effects in dynamics of large reactive systems.

Quantum effects in dynamics of nuclei. Quantum-mechanical effects in molecular dynamics are essential for accurate description and understanding of many chemical processes, such as those in surface reactions, photochemistry, in interactions of molecules with electric field, in chemistry of polymers, clusters and liquids. QM effects are the most pronounced in processes involving atomic and molecular hydrogen including reactions in enzymes, other biomolecular environments and nanomaterials. For example the isotope effects in water are manifested in such basic properties as melting point, which is 3.82C for deuterated water, and the temperature of maximum density in liquid state, which is 4C for water and 11.2C for deuterated water. The exact methods of solving the time-dependent Schrodinger equation based on the grid or basis function representation are unfeasible for systems beyond 10-12 degrees of freedom, because of the exponential scaling of numerical efforts with the system size. In contrast, methods of molecular dynamics, based on classical trajectories are routinely applied to high-dimensional systems of hundreds of atoms, but they have two fundamental limitations: (i) the Born-Oppenheimer separation of motion of electrons and nuclei resulting in a single electronic surface dynamics and (ii) the classical motion of nuclei. Both issues can be resolved by doing dynamics simulation with quantum trajectories. Our theoretical work is guided by the ultimate goal -- to study dynamics of complex molecular systems using an accurate and efficient method which incorporates the quantum effects and is compatible with classical molecular dynamics. Possible applications include proton transfer processes in enzymes and other biomolecular environments and incoherent electron transport in open quantum systems, such as molecular electronic devices.

Quantum or Bohmian trajectories. The time-dependent Schrodinger equation can be recast in terms of the wavefunction amplitude and phase associated with the trajectories evolving in time according to Hamilton's equations of motion. All quantum effects are expressed through the action of quantum potential dependent on the amplitude and its derivatives, acting on a trajectory in addition to the external "classical" potential. For general problems, the exact determination of the quantum potential is at least as difficult as the solution of the standard Schrodinger equation, but the quantum trajectory formulation provides a convenient starting point for approximation of the "quantum" quantities which are small in the semiclassical limit of heavy particles such as nuclei. We develop global approximations to the quantum potential, which capture dominant quantum effects, such as zero-point energy, tunneling, wavepacket bifurcation, in a computationally efficient manner. Long-time (picoseconds) zero-point energy description is of special importance in condensed phase (system interacting with the environment). Current work extends the quantum trajectory formalism to evolution under the Boltzmann operator, which enables direct computation of thermal reaction rate constants from trajectory dynamics. High-dimensional parallel quantum trajectory code with on-the-fly force calculations (DFTB) is under development.

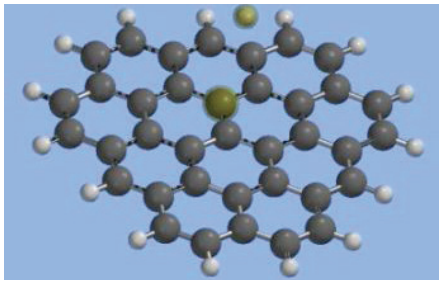

Fig.2: Interaction of hydrogen with graphene. Graphene is modeled as a flat $C_{37}H_{15}$ molecule. We find that adsorption of the hydrogen atom colliding with $C_{37}H_{15}$ is significantly modified by the quantum corrections influencing dynamical behavior of the graphene "flake".

Proton transfer in soybean lypoxygenase-1. Quantum nature of nuclear motion can be crucial for reactions in condensed phase processes, e. g. proton transfer via tunneling has been experimentally identified as a rate-determining step for SLO-1. We are employing trajectory dynamics to assess importance of quantum tunneling in this system, which is representative for proton transfer in biological environments. Unlike exact quantum methods, this approach allows quantum motion of some nuclei to be explicitly included into the simulation.

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Garashchuk, S.; Jakowski, J.; Wang, L.; Sumpter, B. G. Quantum Trajectory-Electronic Structure Approach for Exploring Nuclear Effects in the Dynamics of Nanomaterials. *J. Chem. Theory and Comp.* **2013**, 9,5221-5235

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Garashchuk, S. Calculation of reaction rate constants using approximate evolution of quantum trajectories in imaginary and real time. *Chem. Phys. Lett.* **2010**, 491, 96–101

Garashchuk, S.; Rassolov, V. A.; Schatz, G. C. Semiclassical nonadiabatic dynamics based on quantum trajectories for the O(3P, 1D)+H2 system. *J.Chem. Phys.* **2006**, 244307

SCOTT R. GOODE

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Distinguished Professor, South Carolina Honors College, University of South Carolina, 1986; Amoco Foundation Outstanding Teaching Award, University of South Carolina, 1991; Michael J. Mungo Award for Excellence in Undergraduate Teaching, University of South Carolina, 1998; College of Science and Mathematics Undergraduate Student Advisor of the Year Award, University of South Carolina, 1998; Ada B. Thomas Outstanding Faculty Advisor Award, 2000; S.C. Section ACS Distinguished Service Award, 2009; University of South Carolina Distinguished Service Award, 2013.; South Carolina Honors College Core Faculty, 2014-2016

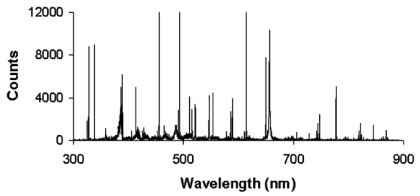

Figure 2. Typical LIBS spectrum

Research Areas: Analytical atomic spectroscopy; plasma spectroscopy; laser atomization; chemical instrumentation; automated and interactive computer control over analytical experiments; environmental analytical chemistry; analytical chemistry of radioactive wastes.

Research in modern analytical chemistry is research in understanding measurements, their accuracy, their precision, and their sources of errors. The analytical chemist oversees the entire process that transforms physical and chemical information, like concentration, into a form meaningful to scientists—a number. The goal of the analytical chemist is to produce the "best," or optimum, measurement. But in order to optimize the measurement, the sources of errors and imprecision of each step in the measurement process must be known. We are currently studying microwave induced plasmas, inductively coupled plasmas, and laser induced plasmas to learn the fundamental plasma processes and to use them as excitation sources in atomic spectroscopy.

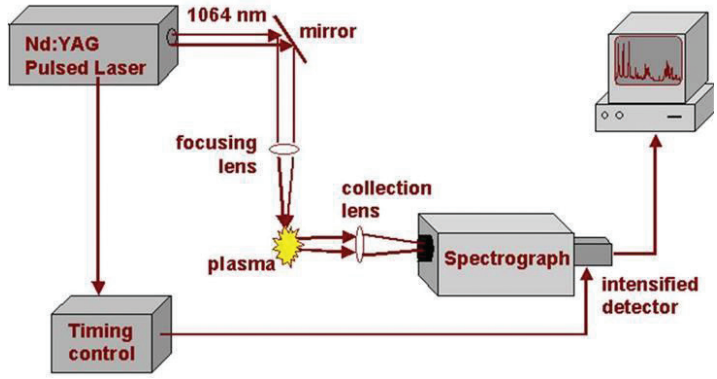

Figure 1. Block diagram of LIBS experiment

The Laser Induced Breakdown Spectroscopy (LIBS). LIBS uses a tightly focused laser beam to vaporize a sample and form a plasma. This relatively new method has many advantages since it can use gas, liquid, or solid samples and is amenable to remote analysis via fiber-optic link. For LIBS to realize its full potential, the events leading to the generation of the optical signal must be studied and understood. One of the most important questions facing the users of this (and of any) analytical tool is whether the sample matrix influences the analytical results. If the analysis is matrix independent, then 2.0 percent lead in paint produces the same signal as 2.0 percent lead in steel. Although the matrix effect could possibly be studied empirically, fundamental studies of the laser induced breakdown spectroscopy provide a much more organized basis to answer this and many other questions. Such work is in progress in our laboratory.

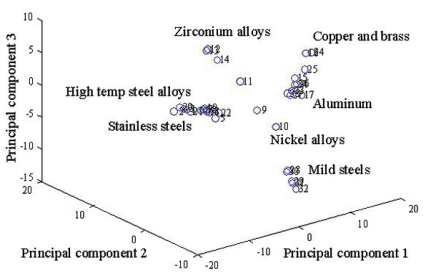

Figure 3. Identification of alloys by principal component analysis of their LIBS spectra

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Dockery, C. R.; Pender, J. E.; Goode, S.R. Speciation of Chromium via Laser-Induced Breakdown Spectroscopy of Ion Exchange Polymer Membranes. *Appl. Spectrosc.* **2005**, 59(2), 252–257.

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Goode, S.R. Influence of the Isotopic Composition of Standards on the Accuracy of Atomic spectrometry. *Appl. Spectrosc.* **2001**, 55, 1225–1228.

Goode, S.R.; S.L. Morgan, R. Hoskins, and A. Oxsher. Identifying alloys by laser-induced breakdown spectroscopy with a time-resolved high resolution echelle spectrometer. *J. Anal. At. Spectrom.* **2000**, 15, 1133–1138.

ANDREW GREYTAK

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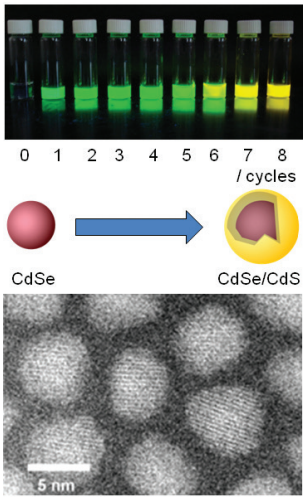
B.S., 2000, Massachusetts Institute of Technology; Ph.D., 2006, Harvard University; Postdoctoral, 2006–2010, Massachusetts Institute of Technology.

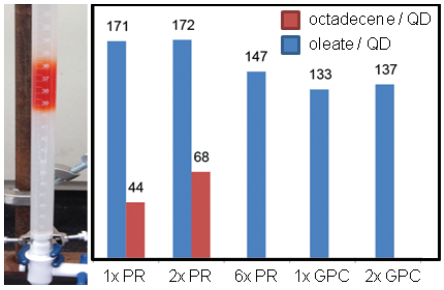
Sustainable Carolina Curriculum Award, 2013; ACS-CEI Award for Incorporating Sustainability into Chemistry Education, 2014.

Research Areas: The Greytak lab explores physical and materials chemistry at the liquid-solid interfaces of semiconductors.



Core/shell structures can increase the brightness of QDs as fluorophores, making them of interest for many applications including bioimaging. Bottom: Scanning transmission electron microscope image of CdSe/CdS core/shell QDs recorded at USC.

A strong inspiration for this work is the opportunity to impact fields including energy conversion, energy storage, and bioimaging, with current interest in understanding how the properties of semiconductor nanostructures (colloidal nanocrystals, catalytically-synthesized nanowires, and heterostructures) can be modified by controlling the chemistry at their surfaces.



Core/shell structures can increase the brightness of QDs as fluorophores, making them of interest for many applications including bioimaging. Bottom: Scanning transmission electron microscope image of CdSe/CdS core/shell QDs recorded at USC.

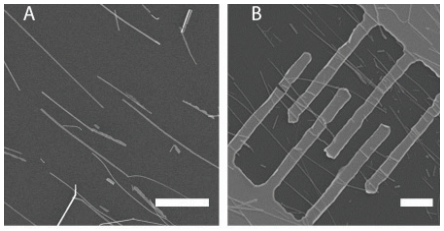
Crystalline materials with nanometer-scale physical dimensions often display different properties than bulk crystals of the same compounds, because they are smaller than characteristic length scales for light absorption and scattering, excited electronic states, and charge transport (conductivity). This is most readily seen in the size-dependent absorption and emission spectra of fluorescent semiconductor nanocrystal "quantum dots."

Synthetic control of nanocrystal and nanowire growth – Nanomaterials are typically larger than molecular compounds and require different methods of growth that focus on achieving a narrowly-distributed ensemble of particles with similar properties. It is often advantageous to distinguish the nucleation process that defines the number and core dimensions of nanostructures, from growth processes that elaborate the existing structures but in which nucleation is not desired.

We employ wet chemistry to form colloidal nanocrystals such as quantum dots. The surfaces of NCs necessarily include regions that do not share the same symmetry with respect to the crystal lattice and are therefore structurally distinct. A current focus of our work is to better understand mechanisms of shell growth in semiconductor nanocrystals, with a goal of enabling the rational design of anisotropic nanocrystals for use in sensors, actuators, and solar cells.

One-dimensional semiconductor nanowires (NWs) can be synthesized by using a catalyst nanoparticle to direct growth in only one crystal direction – and can be synthesized "dry" using vapor-phase precursors. The solvent-free vapor-liquid-solid (VLS) growth method provides the thermal budget to achieve low bulk defect densities, so that carrier mobilities can approach bulk values; this can decrease the series resistance of solar cells.

Surface analysis and ligand exchange chemistry – Interactions of adsorbed molecular layers (ligands) with nanocrystal surfaces are used to control synthesis, solubility, specific and nonspecific biological interactions of fluorescent QD probes, and the conductivity of deposited films. Unfortunately, standard measures such as relative free energies of binding or relative enthalpies (heats) of binding among ligand types have proven difficult to obtain for nanocrystal-ligand interactions. A persistent challenge for colloidal QDs has been to prepare samples that have well-characterized surfaces and are free of unbound ligands.



We use photolithography to pattern microfabricated electrodes for transport measurements on semiconductor nanowires, and to pattern microfluidic structures for in-situ measurements.

We have recently introduced gel permeation chromatography (GPC) as an effective tool in preparing QDs for subsequent use in surface analysis studies, or as biocompatible fluorophores via ligand exchange.

Imaging, spectroscopy, and electronic transport – We use electron and optical microscopy, spectroscopy, and electronic transport measurements to explore the role of the surface in dictating the properties of semiconductor nanostructures such as nanowires and colloidal nanocrystals. Both NCs and NWs are of interest for solar energy capture in photovoltaic or photocatalytic systems as they can absorb sunlight at energies above their bandgaps, can be deposited on diverse and inexpensive substrates, and exhibit large junction areas that could increase the rate at which absorbed light is captured as separated charges.

Representative Publications

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Greytak, A. B.; Allen, P. M.; Liu, W.; Zhao, J.; Young, E. R.; Popović, Z.; Walker, B. J.; Nocera, D. G.; Bawendi, M. G. Alternating layer addition approach to CdSe/CdS core/shell quantum dots with near-unity quantum yield and high on-time fractions. *Chem. Sci.* **2012**, 3, 2028–2034.

Liu, W.; Greytak, A. B.; Lee, J.; Wong, C. R.; Park, J.; Marshall, L. F.; Jiang, W.; Curtin, P. N.; Ting, A. Y.; Nocera, D. G.; Fukumura, D.; Jain, R. K.; Bawendi, M. G. Compact Biocompatible Quantum Dots via RAFT-Mediated Synthesis of Imidazole-Based Random Copolymer Ligand. *J. Am. Chem. Soc.* **2010**, 132, 472–483.

Greytak, A. B.; Barrelet, C. J.; Li, Y.; Lieber, C. M. Semiconductor nanowire laser and nanowire waveguide electro-optic modulators. *Appl. Phys. Lett.* **2005**, 87, 51103.

Greytak, A. B.; Lauhon, L. J.; Gudiksen, M. S.; Lieber, C. M. Growth and transport properties of complementary germanium nanowire field-effect transistors. *Appl. Phys. Lett.* **2004**, 84,4176–4178.

MYTHREYE KARTHIKEYAN

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B.Sc. Honors Biochemistry, 1993-1996, University of Delhi, Delhi, India; M.Sc. Biochemistry, 1996-1998; Hamdard University, Delhi, India; Ph.D., 2000-2005, University of North Carolina, Chapel Hill, NC (Kerry S Bloom Ph.D.)

Career Development Award for Ovarian Cancer Research (Dept. of Defense), 2009-2012; Tilberis Scholar Award, Ovarian Cancer Research Fund, 2013-2016.

Research Areas: Growth factor-receptor signaling mechanisms and signal transduction pathways, Epithelial and Tumor cell biology including Cell survival mechanisms, Cell migration and invasion biology, Cell adhesion and Mechanobiology.

The overall goal of the lab is two fold: 1) Discover the molecular and cellular basis of cancer initiation and metastasis as controlled by growth factors. Specific emphasis is laid on the TGF-β superfamily of growth factors, their receptors, co-receptors and their crosstalk with the integrin family of cell adhesion receptors in cancer. 2) To translate these discoveries into a source of novel therapeutic targets as well as strategies to reduce cancer incidence and improve/predict patient outcomes.

The transforming growth factor-β (TGF-β) superfamily of growth factors, including the TGF-β ligands, the Bone morphogenetic proteins (BMPs), Activins and Inhibin have physiological roles in regulation of growth, cell differentiation and apoptosis in a cell and context-specific manner. TGFβ family ligands induce phenotypic changes in cancer cells including altered morphology, adhesion, motility and invasive behavior via a signal transduction cascade illustrated in Figure 1 and play dichotomous roles in cancer progression switching from tumor suppressors to tumor promoters.

Understanding the mechanism of this dichotomy of TGF-β superfamily function remains a fundamental problem in the cancer biology field and affects our ability to target these pathways in various pathologies.

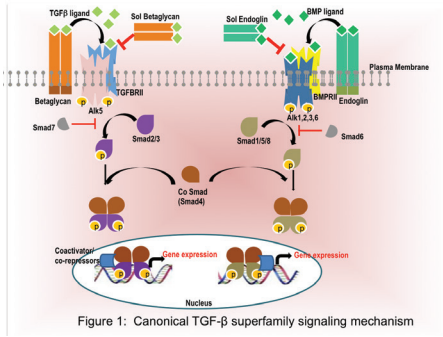


Figure 1: Canonical TGF-β superfamily signaling mechanism

Three core research areas include:

- Role of integrins in regulating TGF-β's effects on carcinogenesis. We have recently determined that TGF-β coreceptors traffic with integrins that impacts their subcellular distribution in cells and cancer tissues. Emphasis will be laid on the intersection of TGF-βand BMP signaling and integrin biology in the context of gynecological cancers, ovarian and breast cancer.
- BMP's are emerging as regulators of breast and ovarian physiology. The aim is to determine the contribution of BMP's in cell survival in ovarian and breast cancer.
- Defining the intersection between growth factor/ biochemical signals and mechanical signals received by cells as the extracellular matrix environment changes in disease. Specifically, the lab investigates how changes in the TGF-β pathways during epithelial to mesenchymal transition may act as a mechanism utilized by cancers to evade mechanical cues to impact cancer cell behavior in breast and ovarian cancer.

Mechanistic studies will be conducted in cell line models of cancer either in two dimension (Figure 2), or in specialized three dimensional organotype culture models (Figure 3).

Identified mechanisms will be translated into preclinical work using small molecule inhibitors, TGF-β antibodies and chemotherapeutic agents in xenograft models and transgenic mice to determine invivo impact.

Figure 2: Two Dimensional Cell spreading

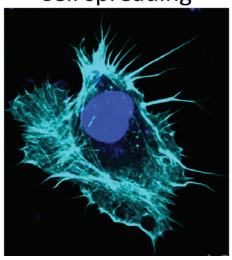
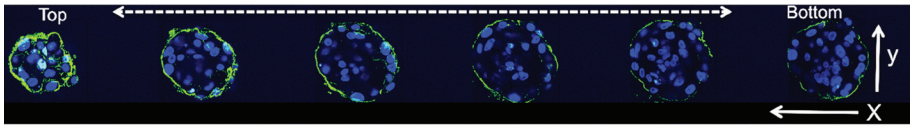


Figure 3: Three Dimensional Model using mammary epithelial cells



Representative Publications

Knelson[1,4], E. H.; Gaviglio1, A. L.; Tewari1[4], A. K.; Armstrong[2], M. B.;Karthikeyan[3], M.; Blobe, G. C. The type III TGF-beta receptor promotes FGF2-mediated neuronal differentiation in neuroblastoma. *JCI* 2013 in press (equal contribution senior author).

Oh, S. Y.; Knelson, E. H.; Blobe, G.C.; Mythreye, K. TβRIII regulates filopodial formation through direct interaction with Cdc42 and Cdc42-mediated IRSP53: NWASP complexes. *Biochem. J.* **2013**, Jun 10 [Epub ahead of print].

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Pan, C. C.; Bloodworth, J. C.; Karthikeyan, M.; Lee, N. Y. Endoglin Inhibits ERK-induced c-Myc and Cyclin D1 Expression to Impede Endothelial Cell Proliferation. *Biochem. Biophys. Res. Comm.* **2012**, 424(3), 620-3. Epub 2012 Jul 10.

Karthikeyan, M.; Knelson, K. E.; Gatza, C. E.; Gatza, M.L.; Blobe, G.C.; TβRIII/β-arrestin2 regulates integrin α5β1 trafficking and function during epithelial cell adhesion. *Oncogene.* **2012**, May 7. DOI: 10.1038/onc.2012.157. [Epub ahead of print].

Swaminathan, V.; Karthikeyan, M.; O'Brien, T. E.; Berchuck, A.; Blobe, G. C.; Superfine, R. Mechanical stiffness grades metastatic potential in patient tumor cells and in cancer cell lines. (equal first author) *Cancer Research* **2011** Aug 1; 71(15):5075-80. Epub 2011 Jun 3.

Lambert, K. E.; Huang, H; Karthikeyan, M.; Blobe, G.C.;The type III transforming growth factor-β receptor inhibits proliferation, migration, and adhesion in human myeloma cells. *Mol. Biol. Cell* **2011** Mar 16.

Karthikeyan, M.; Blobe, G.C.; The type III TGFbeta receptor regulates directional migration: new tricks for an old dog. *Cell Cycle.* **2009**, 8(19), 3069-70.

Karthikeyan, M.; Blobe, G.C. Proteoglycan signaling co-receptors: roles in cell adhesion, migration and invasion. *Cell Signal* **2009**, 21(11), 1548-58.

Karthikeyan, M.; Blobe, G.C. The type III TGF-beta receptor regulates epithelial and cancer cell migration through beta-arrestin2-mediated activation of Cdc42. *Proc. Natl. Acad. Sci. U S A.* **2009**, 106(20), 8221-6.

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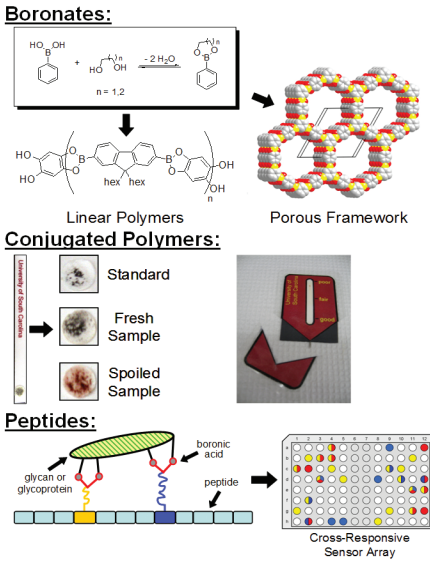
B.S., 1993, St. Lawrence University; M.Ed., 1997, St. Lawrence University; Ph.D., 2000, University of Texas at Austin.

Research Corporation Research Innovation Award, 2004-2009; Distinguished Undergraduate Research Mentor Award, 2007; Golden Key Faculty Award for Creative Integration of Research and Teaching, 2007; Michael J. Mungo Undergraduate Teaching Award, 2009; Mortar Board Excellence in Teaching Award, 2012



Research Areas: Molecular recognition, supramolecular chemistry, sensors, materials, bio-organic, physical organic.

The overriding goal in our lab is to understand and predictably control how molecules interact in order to develop new self-assembled materials for real world applications. For example, these assemblies can serve as diagnostics for cancer and food spoilage, as nano-porous materials for gas storage and separation, as novel conjugated polymers for use in OLEDs and PVs, and as new age plastics.

Students are involved in the design, synthesis, and analysis phases for each project. Computational methods are often used to aid in molecular design. Organic synthesis provides the foundation to build-in the interactions that control the assembly process and ultimately define the materials' properties. Finally, analytical methods (e.g. optical spectroscopy, mechanical, electronic) are used to assess the assembly performance. Ultimately we enjoy projects where an end use beyond the lab is imaginable (often resulting in patents). With this in mind, the research experience gained in the group is often coupled to a biomedical or engineering component. In our efforts we work with three general types of compounds: boronates, conjugated polymers, and peptides.

Boronates: Novel self-assembling boronate-linked materials have been generated as linear polymers, conjugated materials, and nanoporous covalent organic frameworks (COFs). Given that this interaction is covalent yet reversible, these assemblies form with high fidelity. Boronate ester formation maintains all of the desired attributes of self-assembling materials, including ease of synthesis and dynamic self-repair, while at the same time offering stable, covalently linked materials by a route oftentimes more facile and with higher efficiency than conventional polymer synthesis. Boronate-linked specialty plastics exhibit self-repair capabilities and environmental responsiveness. Conjugated poly(boronate)s serve as novel photonic materials and sensitive sensors. Porous COFs and coordination polymers find utility in separations, sequestration, storage, sensing, and catalysis. We continue to investigate the mechanical, optical, and adsorption properties of these unique materials.

Conjugated Polymers: Using conjugated polymers that interact with small molecules and proteins, we have created cross-reactive "aggregative" sensors whose response is defined by the size, shape, and valency of the analyte. For example, a colorimetric sensing approach has been developed that can produce a response visible to the naked eye to determine the freshness of foods as a function of spoilage. A simple, point-of-use dipstick has been developed to assess food quality in restaurants and at home. Advanced analysis can be used to deconvolute complex samples and simplify the device read-out. Studies to detect analytes such as proteins and small molecule biomarkers produce diagnostics for diseases such as cancer and HIV. This concept also investigates how small molecule additives can tune the electronic properties of the polymer-additive assemblies, for use in photonic applications.

New synthetic protocols, based on post-polymerization modifications, are developed to modularly incorporate diverse functionality. This design allows for the rapid generation of new compounds and screening of properties to identify the most interesting candidates for new photonic and sensory materials.

Peptides: Synthetic lectins (SLs) are created to bind glycans and glycoproteins associated with numerous disease states. Specifically, SLs have identified aberrant glycosylation patterns associated with colorectal and other cancer types. These unique compounds have been used as in vitro diagnostics and hold great potential as in vivo imaging agents and therapeutics.

REPRESENTATIVE PUBLICATIONS

Bicker, K. L.; Sun, J.; Harrell, M.; Zhang, Y.; Pena, M. M.; Thompson, P. R.; Lavigne, J. J. Synthetic Lectin Arrays for the Detection and Discrimination of Cancer Associated Glycans and Cell Lines. *Chem. Sci.* **2012**, 3, 1147-1156. DOI: 10.1039/C2SC00790H.

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Bicker, K. L.; Sun, J.; Lavigne, J. J.; Thompson, P. R. Boronic acid functionalized peptidyl synthetic lectins: Combinatorial library design, selective recognition of glycoproteins, and differentiation of carcinogenic cell types. *ACS Combi. Sci.* **2011**, 13, 232–243.

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THOMAS MICHAEL MAKRIS

ASSISTANT PROFESSOR

makrist@mailbox.sc.edu

B.A., 1996, University of Pennsylvania; PhD, 2003, University of Illinois Urbana-Champaign; Postdoctoral Fellow, University of Minnesota

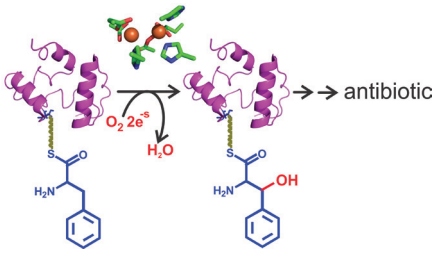
Research Areas: Natural product biosynthesis; non-ribosomal peptides; bioinorganic and biophysical chemistry; oxygen activation; biofuels

My laboratory is interested in the chemical biology of enzymes involved in pharmaceutical biosynthesis and bioenergy production. We are interested in developing tools to understand the detailed molecular mechanisms of these potent catalysts, and ultimately leverage them for the synthesis of natural products of pharmacological or industrial importance. As a result, we utilize a large spectrum of techniques in our studies, ranging from genome mining, molecular biology, metabolic engineering, enzymology, transient kinetics, and biophysical spectroscopy.

Antibiotic Biosynthesis

Peptide-derived natural products, including many antibiotics and chemotherapy drugs, are synthesized by complex multi-modular enzymes termed non-ribosomal peptide synthetases (NRPS). The general peptide structure of a maturing natural product is tailored by accessory enzymes. The antimicrobial and apoptotic activity of natural products are controlled by these modifications, and engenders a unique opportunity to produce new therapeutics or to inhibit the production of microbial virulence factors generated by these pathways in a controlled fashion.

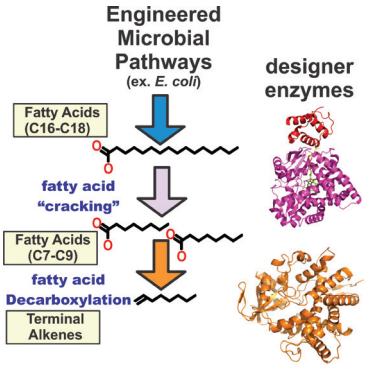
My lab is specifically interested in the molecular mechanisms underlying antibiotic tailoring and exploiting these to make new antimicrobial compounds. We currently study tailoring enzymes that are involved in altering the solubility, peptide structure, glycosylation pattern, and stability of a wide variety of pharmaceuticals. In order to ultimately harness the catalytic versatility of tailoring enzymes, we require a detailed understanding of the molecular recognition events that control the exquisite specificity of a tailoring enzyme to the NRPS and of the detailed catalytic mechanism that occurs at the tailoring enzyme active-site. As each enzyme class is comprised of a unique complex structure and catalytic mechanism, our goal is to develop general paradigms which may enable us to make new compounds in a systematic and combinatorial fashion.



Our examination of non-ribosomal peptide and polyketide biosynthesis pathways affords an excellent opportunity to reveal novel enzymes with unique structures, cofactor requirements, and chemistries. We utilize structural, biochemical, and spectroscopic methods to characterize the catalytic mechanisms of these enzymes and use these as a framework to understood fundamental biochemical processes, such as C-H bond functionalization.

Microbial Hydrocarbon Biosynthesis

There is growing interest in developing biochemical methods to produce compounds with similar properties to petroleum-derived fuels. We are exploring enzymatic routes to produce suitable chain length hydrocarbons from biologically-derived fatty acid precursors, with the ultimate goal of preparing a genetically modified organism capable of efficiently generating these compounds *in vivo*. To this end, we are currently studying a number of enzymes which perform the oxidative cleavage of fatty acids and aldehydes. The chemical mechanisms of these enzymes, largely unknown, present some fascinating deviations from typical oxidative chemistries. For example, one enzyme under study, a cytochrome P450, efficiently catalyzes the oxidative decarboxylation of fatty acids. We are exploring both the substrate selectivity and mechanistic biochemistry (oxygen activation reaction) of this unique reaction. Our goals are to optimize the chain length selectivity of these enzymes, and utilize them in a pathway to efficiently



produce commercially viable drop-in fuels.

REPRESENTATIVE PUBLICATIONS

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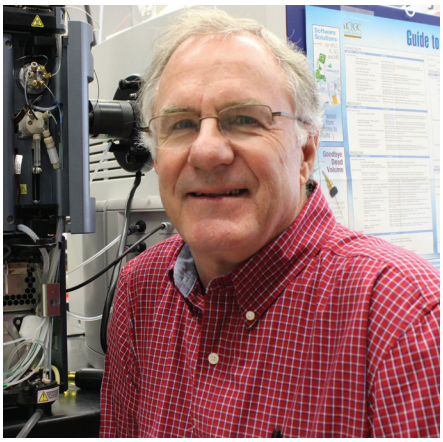

STEPHEN L. MORGAN

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B.S., 1971, Duke University; M.S., 1974, Emory University; Ph.D., 1975, Emory University; Postdoctoral Fellow, 1975–1976, University of Houston.

Distinguished Undergraduate Research Mentor Award, University of South Carolina, May 2007; Sigma Xi Distinguished Lecturer, 2008–2010.

Research Areas: Analytical chemistry. Forensic and environmental analysis using chromatography and mass spectrometry; trace evidence analysis of textile fibers and polymers; rapid spectroscopic visualization of biological stains; noninvasive spectroscopic detection of magnetic tape degradation; chemometrics; analytical pyrolysis.

Our research has targeted diverse areas including analytical separations, mass spectrometry, and spectroscopy. Applications include improvements in forensic fiber analysis, detection of biological stains at crime scenes using thermal imaging in the mid-infrared, and development of rapid noninvasive methods for detection of degraded audio tapes using infrared spectroscopy. These projects in analytical method development are guided by experimental design, optimization, and multivariate pattern recognition methodology.

Forensic imaging in the infrared. Identification of biological fluid stains on materials of evidentiary value (e.g., clothing from a crime scene) is an important in forensic examination. Even minute traces of blood can have probative value because of trace DNA profiling. Luminol spraying is a sensitive technique, but risks diluting and damaging DNA, while alternative light sources are not particularly sensitive. Our continuing collaboration with the Myrick group is designed to develop and characterize mid-infrared imaging techniques for rapid visualization of biological residues at crime scenes. Detection is based on filtered and processed reflectance measurements of absorption from surface stains that contain proteins. While our original work was able to detect 100-200× diluted blood, recent work has extended detection limits to 1000× diluted stains. Designing improved detection modalities, and assessing the influence of environmental contaminants on detection in collaboration with the Forensic Laboratory at the South Carolina Law Enforcement Division, are further research questions we are addressing.

Noninvasive detection of audio tape 'sticky shed' syndrome. Current methods for identifying degraded

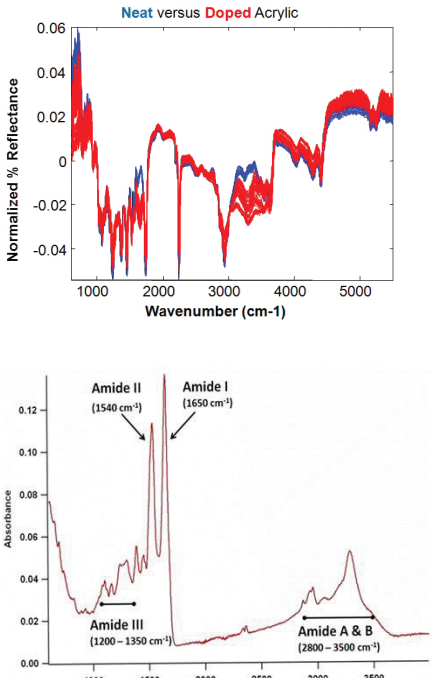

Figure1. (Left): Replicate diffuse reflectance spectra of neat acrylic fabric (blue) and acrylic fabric coated with diluted blood (red); (Right): Infrared spectrum of blood.

tape at museums and archives depend on visual inspection followed by playing, which can irreversibly damage a tape by removing data-containing magnetic particles. Collaborating with Dr. Eric Breitung at the Conservation and Preservation Laboratory of the Library of Congress, we are working to understand the

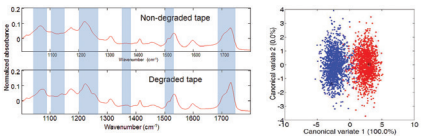

Figure 2. (Left) Relevant features in IR spectra. (Right) Linear discriminant analysis of spectra of playable tapes (blue), and degraded tape (red).

chemical changes in magnetic tapes chemical changes that occur in magnetic tape degradation upon aging using attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR), and direct analysis in real time mass spectrometry (DART-MS). The objective of this work is to develop rapid and noninvasive methods for classification of degraded from playable tapes. Figure 2 shows IR spectra of non-degraded and degraded tapes; spectral features useful for discrimination are shaded. Figure 3 shows discriminant analysis projections for 2660 spectra taken from 133 audio tapes at the Library of Congress; this model produced 97.14% classification accuracy and only misclassified 76 spectra. Recent validation results also produced over 90% classification accuracy for spectra of new audio tape samples not in this training set.

Trace profiling of dyes extracted from textile fibers. Forensic examinations of trace fibers found at a crime scene involve a series of comparisons of one or more fibers of unknown origin, with fibers associated with the circumstances of the crime but whose origin is known. If the null hypothesis of common origin for the two fibers cannot be rejected, the two fibers may have originated from a common source and the evidence may support an association between a victim and a suspect, or between a suspect and the crime scene. Judging statistical or practical significance of a possible 'match' between two fibers is the most challenging issue in forensic fiber analysis because fibers are 'class evidence', for which many similar manufactured items exist. However, the significance of fiber evidence and discrimination are expanded by combinatorial possibilities of fiber types and dyes. We have developed microextraction techniques coupled with UPLC/UV-visible and mass spectrometric methods that enable dye profiling from single fibers as small as 0.5 mm in length. With detection limits in the low picogram range, match exclusions can be made with higher reliability, and "results consistent with" will have increased significance.

Representative Publications

Myrick, M. L.; Morgan, S. L. Infrared specular reflection calculated for polymer films on polymer substrates: Models for the spectra of coated plastics. *Spectroscopy* **2012**, 8, 40-56.

Brooke, H.; Baranowski, M. R.; McCutcheon, J. N.; Morgan, S. L.; Myrick, M. L. Multi-mode Imaging in the Thermal Infrared for Chemical Contrast Enhancement Part 3: Visualizing Blood on Fabrics. *Anal. Chem.* **2010**, 82, 8427-8431.

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Ellison, S. T.; Gies, A. P.; Hercules, D. M.; Morgan, S. L. MALDI-TOF/TOF CID study of polysulfone fragmentation reactions. *Macromolecules* **2009**, 42 (8), 3005–3013.

Stefan, A. R.; Dockery, C. R.; Nieuwland, A. A.; Roberson, S. N.; Baguley, B. M.; Hendrix, J. E.; Morgan, S. L. Forensic analysis of anthraquinone, azo, and metal complex acid dyes from nylon fibers by micro-extraction and capillary electrophoresis. *Anal. Bioanal. Chem.* **2009**, 394, 2077-2085.

Dockery, C. R.; Stefan, A. R.; Nieuwland, A. A.; Roberson, S. N.; Baguley, B. M.; Hendrix, J. E.; Morgan, S. L. Automated extraction of direct, reactive, and vat dyes from cellulosic fibers for forensic analysis by capillary electrophoresis. *Anal. Bioanal. Chem.* **2009**, 394, 2095-2103

MICHAEL L. MYRICK

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B.S., 1985, North Carolina State University; Ph.D., 1988, New Mexico State University.

Army Young Investigator Award, 1992; Outstanding Honors College Professor in the Sciences, University of South Carolina, 1994; Imaging Solution of the Year Award, Advanced Imaging Magazine, 1999; Research Innovation Award, 2004–2009; Gerald Birth Award for Diffuse Reflection, 2012 ; Michael J. Mungo Undergraduate Teaching Award, 2013.

Research Areas: The following sections describe two projects we are currently pursuing.

Spectroscopy of Phytoplankton: Phytoplankton use photosynthesis to produce fixed carbon and are thus key players in pelagic food webs. Many phytoplankton species also form harmful algal blooms (HABs) and can release toxins into the environment that create health problems or kill fish, marine mammals, and humans.

Fluorescence spectroscopy, using excitation and/or emission spectra, provides a noninvasive, non-destructive alternative approach to pigment-based identification, and phytoplankton can be examined intact. The research groups of Prof. Timothy Shaw and Prof. Tammi Richardson (biological sciences) have been working with us to address this problem using the method of multivariate optical computing.

With NSF support, we are developing a field portable imaging flow photometer to capture images and fluorescence excitation data for phytoplankton speciation in seawater. A spinning filter wheel carrying special multivariate optical elements designed and fabricated in our laboratory has now been used in field studies at Martha's Vinyard to detect the classes of phytoplankton is ocean samples. Images of fluorescence tracks of the flowing phytoplankton are decoded using software written here to provide automated analysis of individual organisms. Data

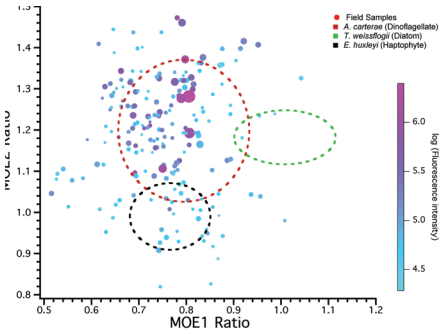

Figure 1. Distribution of signals in field data at Martha's Vinyard Coastal Observatory. Each point represents a single cell. The left and right axes give fluorescence classification signals from multivariate optical elements; color is proportional to the log of intensity for each cell; size of the point represents physical size of the cell. The three dashed ovals are the 95% confidence ellipses for three specific laboratory cultured cells from different classes.

is being correlated with Flow Cytobot data from the laboratory of Dr. Heidi Sosik at Woods Hole Oceanographic Institute to determine instrument sensitivity, cell density, size, classification, and other aspects of the ocean phytoplankton community.

Forensic Infrared Imaging: With support from the National Institute of Justice, we are working in collaboration with the Morgan research group, the S.C. State Law Enforcement Division, and others to develop improved methods for the visualization of biological fluids at crime scenes. Using a silicon

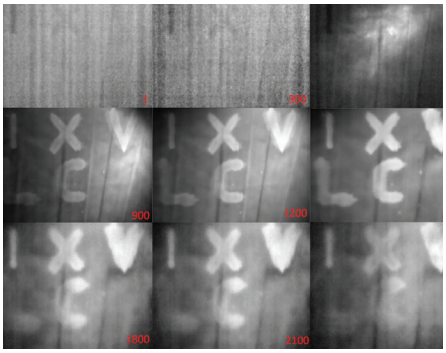

Figure 2 Thermographic images taken from an image sequence during exposure of an acrylic fabric sample to water vapor. The top left and center images are prior to exposure; the symbols visible in subsequent images were formed with different dilutions of blood.

microbolometer camera of the type normally used for detecting blackbody emission from warm objects, we developed hardware and software tools that make it possible to visualize dilute stains on a variety of fabrics.

Most recently we have been exploring a new non-destructive imaging modality that we call latent heat thermography to extend detection limits below one part per thousand dilution for blood and other fluids. In these experiments, water vapor absorption leads to the release of heat that forms a differential thermal image of a latent stain. Specialized hardware is being constructed to optimize the thermal signals and generate both positive and negative differential images. Time-shift and data-processing approaches to formalizing a simple data presentation from a sequence of thermal images are currently being explored, and a beta-test unit is being developed for the forensic laboratory at the State Law Enforcement Division and a commercial partner.

Representative Publications

Swanstrom, J. A.; Bruckman, L. S.; Pearl, M. R.; Simcock, M.N.; Donaldson, K. A.; Richardson, T. L.; Shaw, T. J.; Myrick, M. L. Taxonomic Classification of Phytoplankton with Multivariate Optical Computing, Part I: Design and Theoretical Performance of Multivariate Optical Elements. *Appl. Spectrosc.* **2013**, 67, 220-9.

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Brooke, H.; Baranowski, M.; McCutcheon, J.; Morgan, S. L.; Myrick, M. L. Multimode Imaging in the Thermal Infrared for Chemical Contrast Enhancement. Part 1: Methodology. *Anal. Chem.* **2010**, 82, 8412-20.

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Brooke, H.; Baranowski, M.; McCutcheon, J.; Morgan, S. L.; Myrick, M. L. Multimode Imaging in the Thermal Infrared for Chemical Contrast Enhancement. Part 3: Visualizing Blood on Fabrics. *Anal. Chem.* **2010**, 82, 8427-31.

CARYN E. OUTTEN

ASSOCIATE PROFESSOR, GUY F. LIPSCOMB PROFESSOR OF BIOCHEMISTRY

outten@mailbox.sc.edu

B.S., 1995, College of William and Mary; Ph.D., 2001, Northwestern University; Postdoctoral Fellow, 2001–2005, Johns Hopkins University.

NIEHS Transition to Independent Positions (K22) Award, 2005–08; Presidential Early Career Award for Scientists and Engineers (PECASE), 2009; USC Breakthrough Rising Star, 2011; SC Governor's Young Scientist Award for Excellence in Scientific Research, 2013

Research Areas: Bioinorganic chemistry; protein biochemistry; characterization of cytosolic and mitochondrial redox homeostasis factors; glutathione metabolism; Fe-S cluster biogenesis; structure-function studies of iron homeostasis proteins in prokaryotic and eukaryotic cells

Research in the Outten group is focused on two interconnected projects: (1) identifying the mechanisms by which cells maintain adequate levels of the essential metal iron, and (2) characterizing intracellular factors that control mitochondrial redox balance and combat oxidative stress. We take a multidisciplinary approach to tackle these projects by combining biophysical, biochemical, genetic, and molecular and cell biology techniques. For both projects we primarily use the baker's yeast *Saccharomyces cerevisiae* as a model system since this simple eukaryote is easy to maintain and genetically manipulate in the lab, yet expresses many of the same redox and metal homeostasis systems as human cells.

Project 1: Iron Regulation Mechanisms. Both iron deficiency and iron overload are significant human health issues: iron deficiency is the most common and widespread nutritional disorder in the world, while iron overload disorders are common genetic disorders in the United States. To maintain optimal intracellular iron levels, iron transport and storage is tightly regulated in all eukaryotic cells ranging from yeast to humans. However, there are substantial gaps in our fundamental understanding of iron regulation mechanisms at the cellular and molecular level that require further study, and filling these gaps will be essential for preventing and treating disorders of iron metabolism. Our research program is designed to fill these gaps by providing insight into the basic biology of iron metabolism. In particular, we are focused on monothiol glutaredoxins (Grxs) and BolA-like proteins, which have recently emerged as novel players in iron homeostasis. We are characterizing the structural and functional interactions between these two highly conserved protein families to provide mechanistic insight into their regulatory roles in iron metabolism. We have demonstrated that both yeast and human Grx/BolA proteins form [2Fe-2S]-bridged heterocomplexes with unusual coordination chemistry (Fig 1). In yeast, these complexes inhibit the activity of iron-responsive transcriptional activators that control iron uptake and storage. Overall, our studies are highlighting the essential role that Fe-S clusters play as sensors of cellular iron status in a variety of eukaryotes.

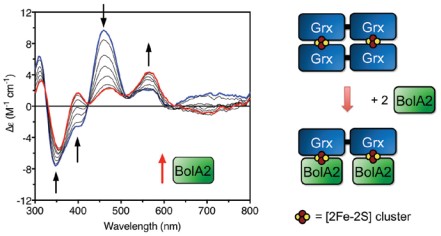

Fig. 1. Circular dichroism spectra of [2Fe-2S] cluster-bound human Glrx3 homodimers (blue) titrated with increasing BolA2 protein (red line = 2-fold excess).

Project 2: Mitochondrial Anti-Oxidant Factors and Redox Control. Iron and redox homeostasis are intimately connected in human health. When left unchecked, excess iron catalyzes formation of reactive oxygen species that disrupt redox homeostasis by oxidatively damaging DNA, proteins, and cell membranes. However, our cells have developed anti-oxidant defense systems that neutralize these reactive by-products and maintain redox balance. *The goal of our second research project is to characterize these anti-oxidant defense systems and redox control pathways, especially within the mitochondrion.* The mitochondrion is a specialized organelle within cells that houses numerous essential functions, including the respiratory machinery

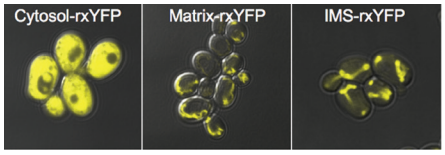

Fig. 2. Fluorescence microscopy images of yeast cells expressing cytosol, matrix, or IMS redox sensors.

responsible for cellular energy production. Consequently, disruption of mitochondrial redox balance contributes to a host of human disorders, including cancer, neurodegenerative diseases, and aging. A better understanding of the factors controlling mitochondrial oxidative stress and redox homeostasis is required for developing therapies to treat mitochondrial disease and dysfunction. To better characterize redox control pathways in mitochondria, we have targeted green fluorescent protein (GFP)-based redox sensors to the intermembrane space (IMS) and matrix of yeast mitochondria to provide a readout of the subcellular redox environment in live cells (Fig. 2). These sensors equilibrate with local glutathione (GSH) pools and register thiol redox changes via disulfide bond formation. This approach allows us to separately monitor the redox state of the matrix and the IMS, providing a more detailed picture of redox processes in these two compartments. Our long-term goal is to characterize the subcellular impact of environmental and genetic factors on thiol redox homeostasis to more fully understand their effects on human health and disease.

REPRESENTATIVE PUBLICATIONS

Poor, C. B.; Wegner, S. V.; Li, H., Dlouhy, A. C.; Schuermann, J. P.; Sanishvili, R.; Hinshaw, J. R.; Riggs-Gelasco, P. J.; Outten, C. E.; He, C. Molecular mechanism and structure of the Saccharomyces cerevisiae iron regulator Aft2. *Proc. Natl. Acad. Sci. U.S.A.* **2014**, 111, 4043-8.

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Toledano, M. B., Delaunay-Moisan, A., Outten, C. E., Igbaria, A. Functions and cellular compartmentation of the thioredoxin and glutathione pathways in yeast. *Antioxid. Redox Signal* **2013**, 18, 1699-711.

Bouldin, S. D., Darch, M. A., Hart, P. J., Outten, C. E. Redox properties of the disulfide bond of human Cu,Zn superoxide dismutase and the effects of human glutaredoxin 1. *Biochem. J.* **2012**, 446, 59-67.

Li, H., Outten, C. E. Monothiol glutaredoxins and BolA-like proteins: [2Fe-2S] binding partners in iron regulation. *Biochemistry* **2012**, 51, 4377-89.

F. WAYNE OUTTEN

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DISTINGUISHED PROFESSOR

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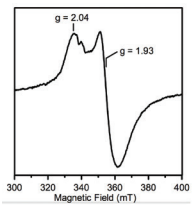
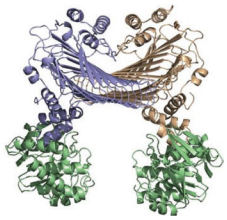
B.S., 1995, College of William and Mary; Ph.D., 2001, Northwestern University; Postdoctoral Fellow, 2001–2005, National Institutes of Health.

Research Corporation Cottrell Scholar, 2008-2010; USC Breakthrough Rising Star, 2012

Research Areas: Microbial metal metabolism, bioinorganic chemistry, microbial physiology, and microbial genetics; biochemical mechanisms of Fe-S cluster assembly; characterization of transition metal acquisition, trafficking, and storage systems and their transcriptional and post-transcriptional regulation during environmental stress.

Metal Trafficking and Metal Cofactor Assembly Under Stress Conditions: My broad research goal is to understand how homeostasis of essential transition metals is maintained in response to environmental stresses. Due to their unique chemical properties, transition metals such as





copper, iron, and zinc are critical cofactors in the active sites of enzymes and as structural components in proteins. However, many of these essential metals are toxic when present in excess, indicating a requirement for the cell to maintain a fairly narrow intracellular concentration of each metal. In addition, metal metabolism may be altered by environmental stress through multiple mechanisms. Cells can adjust transport and storage of the metal in response to the stress, either through increased uptake, efflux, or expression of metal storage proteins. The metal or metal cofactor may be directly modified, for instance by oxidation or reduction, leading to a subsequent change in reactivity, ligand affinity, or bioavailability. Conversely, the proteins or other biomolecules that interact with the metal or metal cofactor may themselves be altered by the stress, causing a change in metal metabolism such as release of metal from an active site. Defining the biochemical strategies used by organisms to maintain metal homeostasis under stress will provide insight into critical areas ranging from bacterial pathogenesis to human disease.

The suf pathway and Fe-S cluster assembly under stress: Fe-S clusters, which contain inorganic sulfur and iron, play key roles in electron transport, as active site cofactors in TCA cycle enzymes, and as exquisite sensors of oxygen and oxygen radicals in stress-responsive transcription factors. However, Fe-S clusters are perturbed by multiple stress conditions. During oxidative stress, superoxide anion ($O_2^{\bullet-}$) can damage 4Fe-4S clusters leading to cluster degradation and release of iron. Therefore, Fe-S clusters are assembled in vivo via intricate biosynthetic pathways. The Fe-S cluster assembly pathway encoded by the sufABCDSE operon is required to assemble Fe-S clusters during iron starvation or oxidative stress, conditions known to disrupt Fe-S clusters in vivo. To determine the biochemical mechanisms used by the suf pathway to achieve this feat, we have purified all six of the suf-encoded proteins. We have found that SufB, SufC and SufD, co-purify as a stable complex. This three-protein complex interacts with the SufE protein to dramatically enhance sulfur donation by the SufS cysteine desulfurase enzyme. SufE acts as a sulfur transfer partner and together with the SufBCD complex, which comprises a novel sulfur transfer pathway for Fe-S cluster assembly under stress conditions. Further genetic, regulatory, and biochemical analysis will elucidate how the suf gene products are adapted to acquire iron and sulfur for construction of Fe-S clusters during iron starvation and oxidative stress.

Metal-responsive Gene Regulation: Transition metal homeostasis is a key process for all forms of life. Metal homeostasis can be disrupted by a variety of environmental or genetic factors. For example, oxygen can alter the oxidation state of some transition metals, such as iron and copper, thereby altering their bioavailability and toxicity. In addition, the requirement for multiple transition metals for correct cell function can be problematic if some transition metals compete with each other for binding to similar protein active sites. Iron is critical for growth due to the need for iron in cofactors like heme and iron-sulfur (Fe-S) clusters. However, iron has limited bioavailability in the environment and iron homeostasis is disrupted by oxidative stress. Iron can also be disrupted by excess levels of other metals, such as cobalt and copper, that compete with iron for incorporation into Fe-S clusters. Under anaerobic conditions in bacteria, iron is combined with nickel in the active sites of the Ni-Fe hydrogenase family of enzymes. During anaerobic growth bacteria increase nickel uptake to provide it for hydrogenase maturation. We have found that excess nickel is toxic to E. coli in part due to disruption of iron homeostasis. We have also identified a transcription factor YqjI that regulates iron homeostasis genes in response to cellular nickel accumulation under anaerobic conditions. YqjI is a nickel-dependent metalloregulatory protein that coordinates control of the ferric reductase YqjH in order to balance iron and nickel uptake under anaerobic conditions. We are characterizing the biochemical mechanism for nickel regulation of YqjI, the transcriptional control of *yqjH* expression, and the in vivo connections between iron and nickel metabolism under anaerobic conditions.

Representative Publications

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Dai, Y. ; Outten, F. W. The E. coli SufS-SufE sulfur transfer system is more resistant to oxidative stress than IscS-IscU. *FEBS Lett.* **2012**, 586(22), 4016-4022.

Chahal, H.K.; Outten, F.W. Separate Fe-S scaffold and carrier functions for SufB2C2 and SufA during in vitro maturation Of [2Fe-2S] Fdx. *J. Inorg. Biochem.* **2012**, 116, 126-134.

Wang, S.; Wu, Y.; Outten, F.W.; Fur and the novel regulator YqjI control transcription of the ferric reductase gene yqjH in Escherichia coli. *J Bacteriol.* **2011**, 193(2), 563-574.

Saini, A.; Mapolelo, D.T.; Chahal, H.K.; Johnson, M.K.; Outten, F.W. SufD and SufC ATPase activity are required for iron acquisition during in vivo Fe-S cluster formation on SufB. *Biochemistry* **2010**, 49(43), 9402-9412.

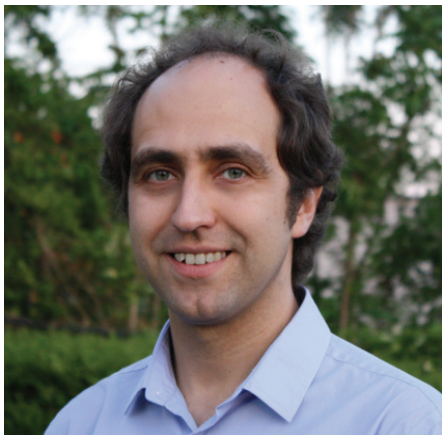
Chahal, H.K.; Dai, Y.; Saini, A.; Ayala-Castro, C.; Outten, F.W. The SufBCD Fe-S scaffold complex interacts with SufA for Fe-S cluster transfer. *Biochemistry* **2009**, 48(44), 10644-10653.

Gupta, V.; Sendra, M.; Naik, S.G.; Chahal, H.K.; Huynh, B.H.; Outten, F.W.; Fontecave, M.; Ollagnier de Choudens, S.; Native Escherichia coli SufA, coexpressed with SufBCDSE, purifies as a [2Fe-2S] protein and acts as an Fe-S transporter to Fe-S target enzymes. *J Am. Chem. Soc.* **2009**, 131(17), 6149-6153.

Wada, K.; Sumi, N.; Nagai, R.; Iwasaki, K.; Sato, T.; Suzuki, K.; Hasegawa, Y.; Kitaoka, S.; Minami, Y.; Outten, F.W.; Takahashi, Y.; Fukuyama, K.; Molecular dynamism of Fe-S cluster biosynthesis implicated by the structure of the SufC2-SufD2 complex. *J. Mol. Biol.* **2009**, 387(1), 245-258.

Wu, Y; Outten, F. W. IscR controls iron-dependent biofilm formation in Escherichia coli by regulating type I fimbria expression. *J. Bacteriol.* **2009**,191(4), 1248-1257.

Layer, G.; Gaddam, S. A.; Ayala-Castro, C. N.; Ollagnier-de Choudens, S.; Lascoux, D.; Fontecave, M.; Outten, F. W. SufE transfers sulfur from SufS to SufB for iron-sulfur cluster assembly. *J. Biol. Chem.* **2007**, 282(18), 13342-13350.



DMITRY PERYSHKOV

ASSISTANT PROFESSOR

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B.S., M.S. Moscow State University, 2004; Ph.D., 2011, Colorado State University; Postdoctoral research associate, 2011-2013, Massachusetts Institute of Technology

Research Areas: Inorganic chemistry and catalysis, organometallics, organic chemistry, solar fuels, carboranes, CO_2 reduction.

Research in the group involves the synthesis of molecular catalysts for activation of important substrates such as dihydrogen, carbon dioxide, and alkenes. Students with interest in catalysis, inorganic, and organometallic chemistry are encouraged to join. Group members will receive a rigorous training in inorganic and organometallic chemistry, catalysis, air-free synthetic methods, and spectroscopic methods. Three main directions are pursued: (i) earth-abundant transition metal complexes supported by multidentate ligands for small molecule activation, (ii) pre-organized frustrated Lewis pairs tolerant to donor functional groups, and (iii) heterometallic complexes for CO_2 photoreduction.

Catalytic Small-Molecule Activation with Transition Metal Complexes Supported by Carboranyl-Based Ligands. The controlled activation of readily available but inert substrates such as hydrocarbons, dihydrogen, dinitrogen, and carbon dioxide has been one of the predominant directions in transition metal chemistry. Rare and expensive precious metals are common components of catalytic systems, and this limits their contribution to the value added product synthesis. Thus, the use of reactive complexes of Earth-abundant metals for catalysis is of great interest. In our group, high-valent transition metal complexes with multiply-bonded ligands active in group-transfer reactions to organic substrates are pursued. The oxo, nitrido, and imido complexes of abundant metals such as V, Mn, Fe, Co, and Ni with multidentate ligands are the main targets. We use boron-rich ligands such as carborane clusters (Figure 1) as a chemically versatile platform for stabilization of reactive transition metal complexes designed for small molecule activation and group transfer. Our research interests are related to the utilization of the unique electronic structure of carboranes for the modification of the reactivity of metal centers.

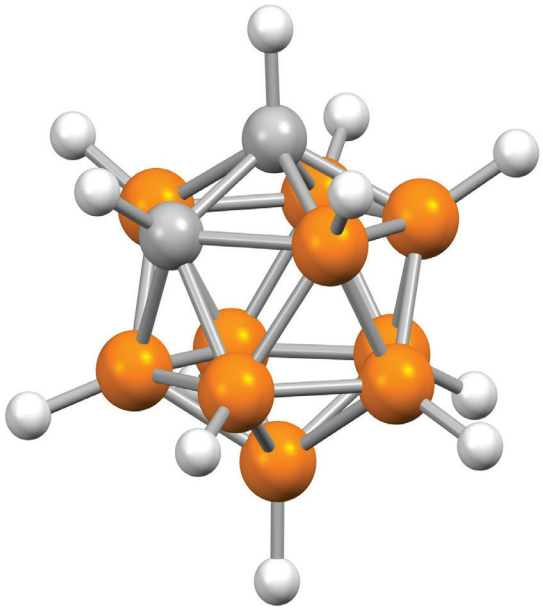

Figure 1. The molecular structure of ortho-carborane cluster.

Pre-Organized Frustrated Lewis Pairs for Small Molecule Activation. Frustrated Lewis pairs (FLPs) are an emerging class of bifunctional intermolecular complexes comprised of sterically encumbered Lewis acidic and basic components. FLPs have demonstrated unique reactivity through metal-free activation of H_2, CO_2, NO, etc. The use of FLPs is generally limited to donor-free substrates due to inactivation of the Lewis acid center of an FLP by basic functionalities. We develop the new types of FLPs that are pre-organized into an intramolecular complex to prevent undesired reactions.

Heterobimetallic molecular complexes for catalytic photoactivation of small molecules. Photocatalytic conversion of common inert molecules such as water and carbon dioxide is a focus of extensive research for solar energy conversion and sustainability. We design molecular heterometallic complexes and study their reactivity in photocatalytic activation of inert molecules such as CO_2.

Representative Publications

Conley, M. P.; Mougel, V.; Peryshkov, D. V.; Forrest, W. P., Jr.; Gajan, D.; Lesage, A.; Emsley, L.; Copéret, C.; Schrock, R. R. A Well-Defined Silica-Supported Tungsten Oxo Alkylidene Is a Highly Active Alkene Metathesis Catalyst. *J. Am. Chem. Soc.* **2013**, 135, 19068–19070.

Cain, M. F.; Forrest, W. P., Jr. ; Peryshkov, D. V.; Schrock, R. R.; Müller, P. Synthesis of a TREN in Which the Aryl Substituents are Part of a 45 Atom Macrocycle. *J. Am. Chem. Soc.* **2013**, 135, 15338–15341.

Peryshkov, D. V.; Forrest, W. P., Jr.; Schrock, R. R.; Smith, S. J.; Müller, P. $B(C_6F_5)_3$ Activation of Oxo Tungsten Complexes That Are Relevant to Olefin Metathesis. *Organometallics* **2013**, 32, 5256–5259.

Peryshkov, D. V.; Schrock, R. R. Synthesis of Tungsten Oxo Alkylidene Complexes. *Organometallics* **2012**, 31, 7278–7286.

Bukovsky, E. V.; Fiedler, S. R.; Peryshkov, D. V.; Popov, A. A.; Strauss, S. H. The Structure of $(H_3O)_2B_{12}F_{12}.6H_2O$ – a CCP Lattice of $B_{12}F_{12}^{2-}$ Anions Intercalated with a Nonplanar Network of O–H. O Connected O_6 Rings. *Eur. J. Inorg. Chem.* **2012**, 208–212.

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Peryshkov, D. V.; Popov, A. A.; Strauss, S. H. Direct Perfluorination of $K_2B_{12}H_{12}$ in Acetonitrile Occurs at the Gas Bubble-Solution Interface and Is Inhibited by HF. Experimental and DFT Study of Inhibition by Protic Acids and Soft, Polarizable Anions. *J. Am. Chem. Soc.* **2009**, 131,18393–18403.

VITALY RASSOLOV

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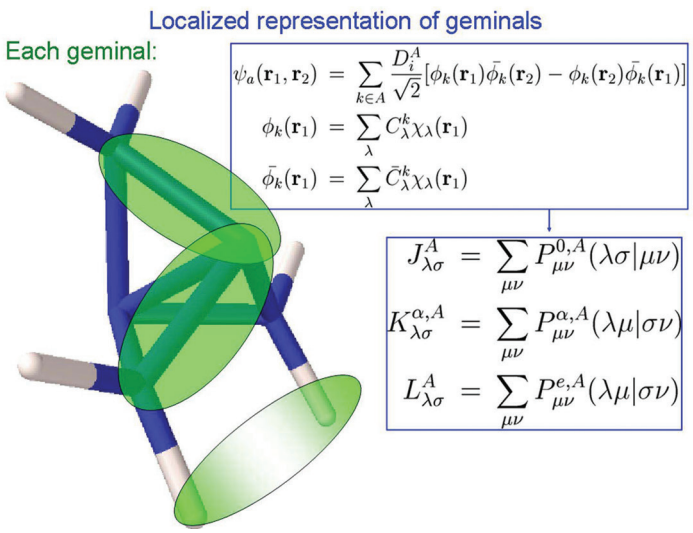

M.S., Physics, 1992, Moscow Institute of Physics and Technology; M.S., Chemistry, 1992, University of Notre Dame; Ph.D., Chemistry, 1996, University of Notre Dame.

Invited Professor, University of Nice, France, 2009.

Research Areas: Quantum chemistry; hyperfine interactions; use of linear operators to describe electron correlation effects in molecules.

Currently my work focuses on three topics.

Geminal Theory. Modern electronic structure methods can be divided into two groups: simple single-reference methods (Hartree-Fock, Coupled Cluster, Kohn-Sham Density Functional Theory) and "custom-made" multireference methods (MCSCF, CASPT2). Single-reference methods work well for equilibrium ground states of not very reactive species, and multireference methods are often computationally expensive and are hard for nontheorists to use. We are developing a new, well-defined method based on geminal representation of the wave function. Its full name is Antisymmetrized Product of Singlet type Strongly orthogonal Geminals (APSSG), and SSG is the shorter acronym. The SSG method is the only practical model that is both variational and size consistent. Its computational cost is only modestly higher than the versatile Hartree-Fock. The target applications of SSG are chemistry of transition metal elements and potential energy surfaces (reaction barriers, bond energies).

Semiclassical Dynamics Based on Quantum Trajectories.
It is well known to theorists that most chemical reactions require quantum description of nuclei due to the effects of tunneling, zero point energy, and non-adiabatic phenomena. It is appealing to describe quantum effects using semiclassical methods. The problem is that modern semiclassical methods are often more expensive than full quantum treatment, and their error is difficult to assess. My group develops a method based on Bohmian trajectories that is very inexpensive at the semiclassical limit, favorably compares to other semiclassical methods (such as Herman-Kluk), and is systematically improvable.

Correlation Operator Approach.
Exact theoretical description of chemical systems is impossible beyond the smallest model systems (this is a so-called NP-hard problem in the computational complexity terminology). The widely popular Density Functional Theory attempts to bypass this problem by modeling chemical systems aiming for adequate accuracy. The underlying theoretical machinery of this modeling mainly comes from solid-state physics. We work on using instead the traditional tools of quantum chemistry, such as linear operators. We seek a universal two-electron operator that can describe electron correlation effects in single determinant wave functions, with sufficient accuracy.

Representative Publications

Adams, R. D.; Rassolov, V.; Zhang, Q. Synthesis and Transformations of Triosmium Carbonyl Cluster Complexes Containing Bridging Aryl Ligands. *Organmetallics* **2012**, 31(8), 2961-2964.

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Rassolov, V. A.; Garashchuk, S. Computational complexity in quantum chemistry. *Chem. Phys. Lett.* **2008**, 464 (4-6), 024109.

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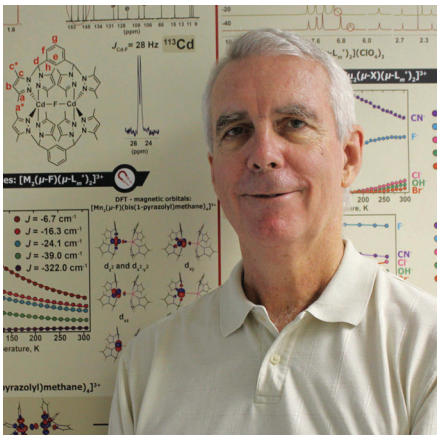
Rassolov, V. A.; Xu, F. Geminal model chemistry. IV. Variational and size consistent pure spin states. *J. Chem. Physics* **2007**, 127 (4),044104.

Garashchuk, S.; Rassolov, V. A. Semiclassical nonadiabatic dynamics of NaFH with quantum trajectories. *Chem. Physics Lett.* **2007**, 446 (4–6), 395–400.



DANIEL L. REGER

CAROLINA DISTINGUISHED PROFESSOR

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B.S., 1967, Dickinson College; Ph.D., 1972, Massachusetts Institute of Technology; Visiting Fellow, Australian National University, 1985, 1994.

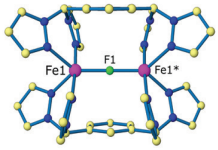
USC Educational Foundation Research Award for Science, Mathematics, and Engineering, 1995; Michael J. Mungo Award for Excellence in Undergraduate Teaching, 1995; Amoco Foundation Outstanding Teaching Award, 1996; Carolina Trustee Professorship, 2000; Michael J. Mungo Award for Excellence in Graduate Teaching, 2003; South Carolina Governor's Award for Excellence in Scientific Research, 2007; University of South Carolina Educational Foundation Outstanding Service Award, 2008; American Chemical Society Outstanding South Carolina Chemist of the Year, 2008; Fellow of the American Association for the Advancement of Science, 2011; Charles H. Stone Award, Charlotte/ Piedmont Section of the American Chemical Society, 2011; Southern Chemist Award, Memphis Section of the American Chemical Society, 2013 .

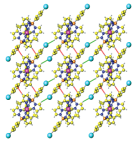
Research Areas: Inorganic chemistry. Synthesis of third generation poly(pyrazolyl)methane and poly(pyrazolyl) borate ligands and ligands containing aromatic groups that form strong π-π stacking interactions; preparation of metal complexes of these ligands that have unusual magnetic and structural properties.

Our group is the leader worldwide in the development of the chemistry of tris(pyrazolyl)methane ligands. These ligands, the neutral analogs of the extensively investigated, isoelectronic tris(pyrazolyl)borate ligands, were not studied extensively prior to our work because they were difficult to prepare. We have now dramatically improved these preparations making the whole family of $HC(3\text{-}Rpz)_3$ (pz = pyrazolyl ring;R = Ph, Pr^i, Bu^t) ligands and $HC(3,5\text{-}Me_2pz)_3$ readily available for the first time. We have functionalized these new ligands to prepared a number of new polytopic ligands (those with multiple pol(pyrazolyl) methane units in a single molecule), a development that represent the first major effort to prepare "third generation" poly(pyrazolyl)methane ligands. Third generation ligands are specifically functionalized at the non-coordinating, "back" position, distal from the metal environment, for the purpose of appending new/ desired functionality into the systems under study while not impacting the direct environment about the metal.

We have developed unusual chemistry of many different metal system with these ligands. A particularly exciting example is the reaction of $M(BF_4)_2$ compounds with Lm resulting in fluoride abstraction leading to the complexes $[M_2(\mu\text{-}F)(\mu\text{-}L_m)2](BF_4)_3$ (see below for M = Fe structure) in which a single fluoride ligand and two Lm molecules bridge the two metal centers. The M = Fe complex shows weakly antiferomagnetic behavior.

In a separate project we have used tris(pyrazolyl) methane ligands to prepare new iron(II) complexes that show very unusual spin properties. The complex

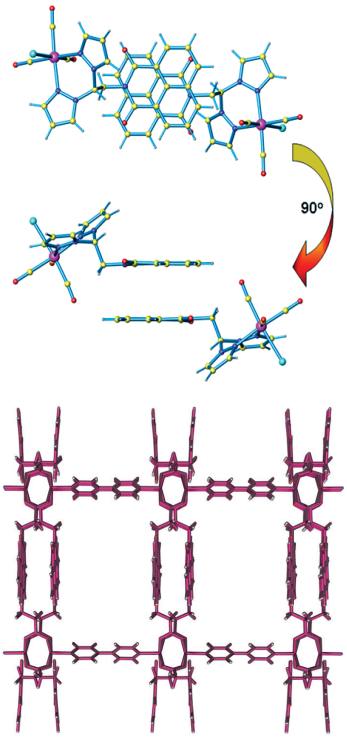




$\{[HC(3,5\text{-}Me_2pz)_3]_2Fe\}(BF_4)_2$ is fully high spin from 350 K to 206 K then undergoes an abrupt spin change to a mixture of high and low spin forms, an unprecedented result. It also undergoes a solid-state phase change at 206 K, a change we have observed for other analogous complexes of first row metals showing that the phase change drives the spin-state change. In recent work we are studying the effects of controlling spin-crossover effects by manipulating the supramolecular structures of the compounds. We have synthesized a new family of "third generation" poly(pyrazolyl)borate ligands. Using these ligands we have been able to show that subtle changes in either molecular or supramolecular structure can greatly influence the spin-crossover behavior of iron(II) complexes. The figure shows the three dimensional structure of one polymorph of

$Fe[(p\text{-}IC_6H_4)B(3\text{-}Mepz)_3]_2$ where the highly organized structure prevents the molecules from undergoing spin crossover at low temperature.

Incorporating the 1,8-naphthalimide group into bis(pyrazolyl)-methane ligands allows the asscoiation of their metal complexes into directionally ordered dimers by strong π-π stacking interactions in both solution and solid-state, as pictured. The incorporation of this π-bonding group into acetate ligands leads to the formation of paddlewheel metalladimers with very unusual supramolecular structures held together by non-covalent forces, as pictured.



REPRESENTATIVE PUBLICATIONS

Reger, D. L.; Pascui, A. E.; Foley, E. A.; Smith, M.D.; Jezierska, J.; Ozarowski, A. Dinuclear Metallacycles with Single M-O(H)-M Bridges [M = Fe(II), Co(II), Ni(II), Cu(II)]: Effects of Large Bridging Angles on Structure and Antiferromagnetic Superexchange Interactions. *Inorg. Chem.* **2014**, 53, 1975-1988.

Reger, D. L.; Leitner, A. P.; Smith, M. D.; Tran, T. T.; Halasyamani, P. S.Homochiral Helical Metal-Organic Frameworks of Group 1 Metals. *Inorg. Chem.* **2013**, 52, 10041-10051.

Reger, D. L.; Pascui, A. E.; Pellechia, P. J.; Smith, M. D. Zinc(II) and Cadmium(II) Monohydroxide Bridged, Dinuclear Metallacycles: A Unique Case of Concerted Double Berry Pseudorotation. *Inorg. Chem.* **2013**, 52, 11638-11649.

Reger, D. L.; Pascui, A. E.; Pellechia, P. J.; Ozarowski, A. NMR Investigations of Dinuclear, Single Anion Bridged Copper(II) Metallacycles: Structure and Antiferromagnetic Behavior in Solution. *Inorg. Chem.* **2013**, 52, 12741-12748.

Reger, D. L.; Pascui, A. E.; Smith, M. D.; Jezierska, J.; Ozarowski, A. Halide and Hydroxide Linearly Bridged Bimetallic Copper(II) Complexes: Trends in Strong Antiferromagnetic Superexchange Interactions. *Inorg. Chem.* **2012**, 51, 7966–7968.

Reger, D. L.; Leitner, A. P.; Smith, M. D. Homochiral Helical Main Group Metal-Organic Frameworks: Potassium. *Inorg. Chem.* **2012**, 51, 10071-10073.

Reger, D. L.; Pascui, A. E.; Smith, M. D.; Jezierska, J.; Ozarowski, A. Dinuclear Complexes Containing Linear M-F-M (M = Mn(II), Fe(II), Co(II), Ni(II), Zn(II), Cd(II)) Bridges: Trends in Structures, Antiferromagnetic Superexchange Interactions and Spectroscopic Properties. *Inorg. Chem.* **2012**, 51, 11820-11836 .

Reger, D. L.; Debreczeni, A.; Smith, M.D. Homochiral, Supramolecular Frameworks Built from a Zinc(II) Tetramer or Cadmium(II) Dimer Containing Enantiopure Carboxylate Ligand Functionalized with a Strong π-π Stacking Stacking Synthon. *Eur. J. Inorg. Chem.* **2012**, 712-719.

SUSAN D. RICHARDSON

ARTHUR SEASE WILLIAMS PROFESSOR OF CHEMISTRY

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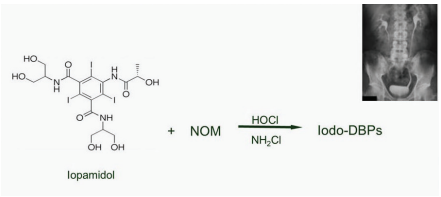
B.S., 1984, Chemistry & Mathematics, Georgia College & State University; Ph.D., 1989, Physical Organic Chemistry, Emory University

Cape Breton University, Sydney, Nova Scotia, Canada, 2006; American Chemical Society Award for Creative Advances in Environmental Science & Technology, 2008; Chemist of the Year, Northeast Georgia Section of the American Chemical Society, 2008; Associate Editor, Water Research, 2009-present; Editorial Advisory Board, Environmental Science & Technology, 2009-present; Editorial Advisory Board, Environmental Science and Pollution Research, 2009-present; Scientific Advisory Committee, NIREAS Cyprus International Water Institute, 2010-present; U.S. EPA, Scientific and Technological Achievement Awards, 2013, 2010, 2009, 2004, 2003, 2001, 2000, 1998, 1997; American Chemical Society (ACS) Expert, Clean Water for the World's Population, 2014-2016; Scientific and Technological Board, European Commission World Joint Programming Initiative (JPI) for 'Water Challenges for a Changing World', 2014-present.

Research Areas: Environmental chemistry; formation of drinking water disinfection by-products (DBPs); emerging environmental contaminants; fate of natural organic matter and environmental contaminants in drinking water and wastewater treatment; linking chemistry and toxicology.



Medical imaging compounds (X-ray contrast media) from wastewater effluents react with chlorine or chloramine in drinking water treatment to form toxic iodo-DBPs.

Introduction: My research focuses mostly on identifying new DBPs in drinking water, determining formation mechanisms, and integrating toxicological characterization with chemical characterization approaches. The overall goal of this research is to solve human health issues surrounding drinking water DBPs. I will also be expanding my work to study and protect ecological health.

Background: Drinking water disinfection was a triumph of the 20th Century, allowing the prevention of many waterborne illnesses, such as cholera and typhoid. However, an unintended consequence of killing harmful pathogens in water is the formation of DBPs in drinking water, many of which have been found to be toxic and/or carcinogenic. Human epidemiologic studies conducted in the U.S. and in other countries have shown increase risk for bladder cancer and the potential for early-term miscarriage and birth defects in some locations, and the DBPs responsible for these effects are currently not known. In addition, people can be exposed to DBPs in swimming pools and spas, and there is interest in what chemicals are formed in these scenarios.

DBPs are formed when disinfectants (e.g., chlorine, chloramines, ozone, and chlorine dioxide) react with naturally occuring organic matter, bromide, and iodide. They can also form through the reaction of disinfectants with anthropogenic contaminants, such as pharmaceuticals and personal care products, hormones, pesticides, and other contaminants. For example, my group made the recent discovery that compounds used for medical imaging (X-ray contrast media) can react with chlorine or chloramines in drinking water treatment to form iodinated DBPs, which are the most toxic DBPs identified to-date. X-ray contrast media are non-toxic to humans in their parent form, and are excreted within ~24 hr. They subsequently enter a wastewater treatment plant and are very resistant to degradation, such that high levels are released to rivers and streams (up to 100 ppb) and can enter drinking water source waters to form these highly toxic DBPs.

This source-to-tap scenario is one of the new research areas of our group, where we are studying the fate of emerging contaminants through wastewater treatment, to drinking water source waters, and transformation in drinking water treatment. Our research is expanding to not only include an emphasis on protecting human health, but also ecological health, as transformation products formed in disinfected wastewater can also adversely impact ecological health. As we understand the formation of these DBPs and transformation products, we can ultimately find ways to remove them or minimize their formation.

Experimental approach: We use gas chromatography (GC)/mass spectrometry (MS) and liquid chromatography (LC)/MS techniques to identify and measure DBPs and other transformation products in drinking water and other treated waters. Mass spectrometry is an ideal analytical tool for measuring trace levels of compounds in complex environmental matrices, and we utilize several different ionization modes as well as high resolution-MS. We also use total organic halogen (TOX) analysis and ion chromatography.

Current research: My current research involves the X-ray contrast media DBP research mentioned above, along with formation of DBPs in desalination treatment and in swimming pools and spas. I am also investigating the effect of free chlorine contact time on the formation of iodo-DBPs from chloramination and continue to collaborate in a European epidemiologic study of DBPs and adverse birth outcomes. I am also interested in helping to solve more recent issues with skin rashes and other respiratory issues that have been associated with chloraminated water.

Representative Publications

Richardson, S. D.; Ternes, T. A. Water Analysis: Emerging Contaminants and Current Issues. *Anal. Chem.* **2014**, 86, 2813-2848.

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Duirk, S. E.; Lindell, C. ; Cornelison,C. C.; Kormos, J.; Ternes, T. A.; Attene-Ramos, M.; Osiol, J.; Wagner, E.D.; Plewa, M. J.; Richardson, S. D. Formation of Toxic Iodinated Disinfection By-Products from Compounds Used in Medical Imaging. *Environ. Sci. Technol.* **2011**, 45 (16), 6845-6854.

Boyd, J. M.; Hrudey, S.E.; Richardson, S.D.; Li, X.-F. Solid Phase Extraction and High Performance Liquid Chromatography Mass Spectrometry Analysis of Nitrosamines in Treated Drinking Water and Wastewater. Trends *Anal. Chem.* **2011**, 30 (9), 1410-1421.

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Richardson, S. D.; Fasano, F.; Ellington, J. J.; Crumley, F. G.;Buettner, K. M.; Evans, J. J.; Blount, B. C.; Silva, L. K.; Waite, T. J.; Luther, G. W.; McKague, A. B.; Miltner, R. J.; Wagner, E. D.; Plewa, M. J. Occurrence and Mammalian Cell Toxicity of Iodinated Disinfection Byproducts in Drinking Water. *Environ. Sci. Technol.* **2008**, 42 (22), 8330-8338.

TIMOTHY J. SHAW

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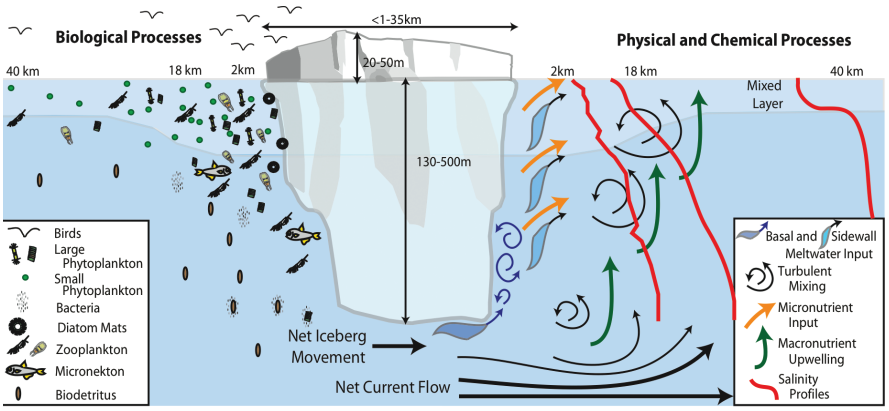
B.S., 1981, California State Polytechnic University; Pomona; Ph.D., 1988, University of California, San Diego, Scripps Institution of Oceanography; Postdoctoral Scholar, Woods Hole Oceanographic Institution - MIT.

Fellow at the Hanse Institute for Advanced Study, Delmenhorst, Germany, 1999; Visiting professor, University of Oldenburg, 2002; Fellow at the Hanse Institute for Advanced Study in Germany for 2010–2011.

(Photo: Dr. Shaw on the icebreaker LM Gould in an Antarctic ice field)

Research Areas: Trace element geochemistry; environmental analytical chemistry; techniques development for trace elements of both anthropogenic and natural origin in the environment; geochemical cycling of trace elements in the environment. My work is focused on identifying factors that control the exchange of trace elements between the dissolved, particulate and biogenic phases in both the marine and fresh water systems. The goal is to identify the processes that control cycling and trophic transfer of trace elements and trace contaminants in the environment. Toward this end, my group routinely measures trace elements and tracers in groundwater, seawater, sediments, particulates (both inorganic and biogenic) and icebergs. In order to make these measurements, we also develop analytical techniques for trace element analysis in aqueous, colloidal, and solid phases and design and build sampling equipment. We maintain a clean room facility, and a radiochemical analysis laboratory that includes multiple coincidence counters for analysis of ^{223}Ra and and ^{224}Ra as well as ^{227}Ac isotopes, and a low level Beta counter for ^{234}Th analysis. We work closely with the departmental elemental mass spectrometry facility that includes two High Resolution Inductively Coupled Plasma Mass Spectrometers (HR-ICP-MS). My group is in the midst of .a program to examine the impact of groundwater mixing and exchange at the terrestrial/ocean interface. Currently, this work is focused on characterizing the processes that lead to the production of Reactive Oxygen Species at the groundwater/seawater interface as a function of the oxidation of Fe(II). This work is part of a combined set of laboratory/field experiments with Dr. John Ferry's research group.



Schematic diagram of the iceberg ecosystem based on the results from previous studies. Biological processes are represented on the left; chemical and physical provesses are represented on the right (from Smith et al., 2013).

We have also participated in several NSF funded projects to evaluate the role of free drifting icebergs as a micronutrient source in the Southern Ocean. This work is part of a large collaborative program with Dr. Ken Smith at the Monterey Bay Aquarium Research Institute (MBARI). These projects involved the measurement of tracers of terrestrial material flux to the Southern

Ocean and requires the development of specialized sampling equipment and new analytical methods. This work is part of a larger effort to characterize mechanisms of atmospheric CO_2 sequestration in the Southern Ocean as a function of climate change (see figure).

Representative Publications

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Swanstrom, J. A.; Bruckman, L. S.; Pearl, M.; Simcock, M.; Abernathy, E., Richardson, T. L.; Shaw, T. J.; Myrick, M. L. Taxonomic Classification of Phytoplankton with Multivariate Optical Computing, Part II: Design and Experimental Protocol of a Shipboard Fluorescence Imaging Photometer. *Appl. Spectrosc.* **2013,** 67(6), 630-639.

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Smith, K. L. Jr.; Sherman, A.D.; Shaw, T.J.; Sprintall, J. Icebergs as Unique Lagrangian Ecosystems in Polar Seas. *Annu. Rev. Mar. Sci.* **2013,** 5, 14.1–14.19.

Vernet, M.; Smith, K. L., Jr.; Cefarelli, A. O.; Helly, J. J.; Kaufmann, R. S.; Lin, H.; Long, D. G.; Murray, A. E.; Robison, B. H.; Ruhl, T. J. Shaw, H. A.; Sherman, A.D.; Sprintall, J.; Stephenson, G. R. Jr.; Stuart, K. M.; Twining, B.S. Islands of ice: Influence of free-drifting Antarctic icebergs on pelagic marine ecosystems. *Oceanography* **2012,** 25(3), 38–39.

Bruckman, L. S.; Richardson, T. L.; Swanstrom, J. A.; Donaldson, K. A.; Allora, M. Jr.; Shaw, T. J.; Myrick, M. L. Linear Discriminant Analysis of Single-Cell Fluorescence Excitation Spectra of Five Phytoplankton Species *Appl. Spectrosc.* **2012,** 66(1), 60-65.

Shaw, T. J.; Raiswell, R. W.; Hexel, C. R.; Vu, H. P.; Moore, W. S.; Dudgeon, R.; Smith, K. L., Jr. Input, composition, and potential impact of terrigenous material from free-drifting icebergs in the Weddell Sea. *Deep-Sea Res. II.* **2011,** 58, 1376–1383.

Shaw, T. J.; Hexel, C. R.; Smith, K. L., Jr.; Sherman, A.D.; Dudgeon, R.; Vernet M.; Kaufmann, R. ^{234}Th –based carbon export around free-drifting icebergs in the Southern Ocean. *Deep-Sea Res. II.* **2011,** 58, 1384–1391.

Smith, K. L., Jr.; Sherman, A.D.; Shaw, T. J.; Murray, A.; Vernet, M.; Cefarelli, A. O. Carbon export associated with free-dri.fting icebergs in the Southern Ocean. *Deep-Sea Res. II.* **2011,** 58, 1485-1496.

KEN D. SHIMIZU

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B.A., 1990, Phi Beta Kappa, Cornell University; Ph.D., 1995, Massachusetts Institute of Technology; NIH Postdoctoral Fellow, 1995–1997, Boston College.

Research Corporation Award, 1994; Mortar Board Teaching Award, 2001; Japan Society for the Promotion of Science Postdoctoral Fellowship Program, 2004; Editorial Advisory for the Journal of Molecular Recognition, 2008; Michael J. Mungo Undergraduate Teaching Award, 2008.

Research Areas: Organic chemistry, supramolecular, physical organic, and polymer chemistries.

Introduction: Research in the Shimizu-group is focused on designing small molecules and polymers for 1) measuring weak non-covalent interactions, 2) sensors and sensor arrays, and 3) molecular devices. Our common strategy in these projects is manipulating shape on the molecular-level, which provides precise control over molecular properties such as recognition, self-assembly, and molecular dynamics.

Project 1. Molecular balances to measure non-covalent interactions. Despite the importance of the weak attractive forces between molecular surfaces in biological systems and materials applications, many of the fundamental aspects of these non-covalent interactions are still not well-understood. To address this problem, we have developed molecular devices to measure and study these weak (< 1 kcal/mol) interactions (Fig. 1). These "molecular balances" have a conformational equilibrium that can be tipped by an intramolecular interaction. Thus, measurement of the conformational ratio provides a sensitive and accurate measure (±0.03 kcal/mol) of these interactions. We have applied our molecular balances to study π–stacking, CH–π, lone pair–π, and cation–π interactions.

Project 2. Molecularly imprinted polymers (MIPs). The molecular imprinting process (Fig. 2) is one of the few methods that can produce synthetic receptors for a specific molecule. MIPs are formed in an efficient one-pot process. Monomers bearing recognition groups are polymerized in the presence of a template molecule. Removal of the template creates binding sites lined with complementary groups. MIPs have applications as synthetic antibodies, catalyst, solid-phase extraction, chiral separations, and sensing. We have developed new imprinting methods that yield more biological-like recognition properties. We have also explored applications of MIPs as versatile and inexpensive components in fluorescent sensor arrays.

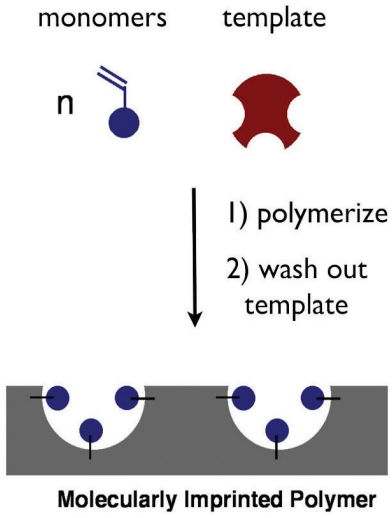

Fig 2. Schematic representation of the molecular imprinting process.

Project 3. Molecular devices. Many important biological functions such as DNA replication, cell division, and motion are carried out by molecular-scale devices. Thus, the development of synthetic molecular devices is an area of great interest. We have designed a series of molecular devices based on the control of the rotation of the $C_{(aryl)}$-$N_{(imide)}$ single bonds. These include molecular breaks, molecular motors, molecular probes, and programmable molecules and polymers with molecular memory. The challenge on the molecular-scale is not to create motion as there is ample kinetic energy. Instead, the problem is to control molecular motion and to interface with macroscale inputs. An example of our molecular devices is shown in Fig. 3. The rate of rotation of this quinoline-succinimide molecular rotor can be controlled by the addition or removal of acid. The protons act as "grease" accelerating the rotation by seven orders of magnitude by allowing the nitrogen and oxygen groups to more easily slip-by each other.

Representative Publications

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Zhang, Y.; Song, D.; Lanni, L. M.; Shimizu, K. D. Importance of Functional Monomer Dimerization in the Molecular Imprinting Process. *Macromolecules* **2010**, 43, 6284-6294.

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Carroll,W. R.; Pellechia, P.; Shimizu, K. D. A Rigid Molecular Balance for Measuring Face-to-Face Arene–Arene Interactions. *Org. Lett.* **2008**, 10, 3547-3550.

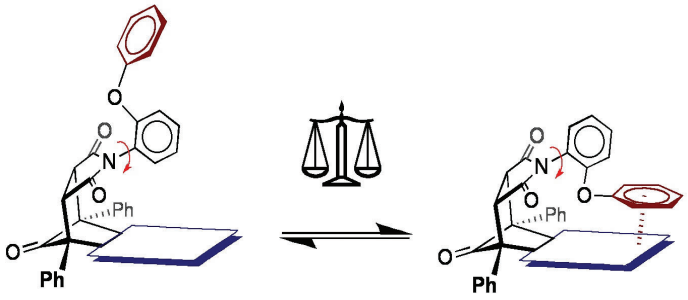

Fig. 1. A molecular balance for studying π-stacking interactions.

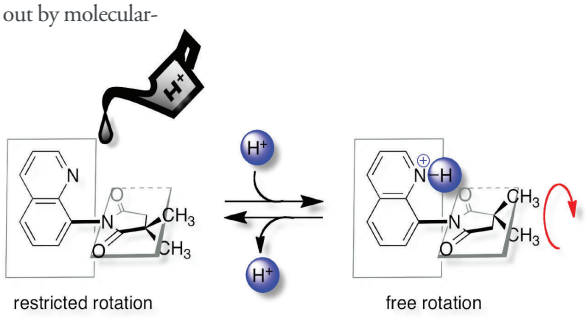

Fig. 3. Acceleration of a molecular rotor using "proton grease".

LINDA SHIMIZU

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B.A., 1990 Wellesley College; Ph.D. 1997, Massachusetts Institute of Technology; NIH Postdoctoral Fellow, 1997-1998, Massachusetts Institute of Technology; Research Assistant Professor, University of South Carolina, 1999-2005, Assistant Professor, University of South Carolina 2005-2011.

USC Breakthrough Rising Star, 2011; ACS WCC Rising Star Award, 2013

Research Areas: Organic, Supramolecular Chemistry, Nanomaterials, Bioorganic, Organic Photochemistry, and Crystal Engineering

Research Summary: We are interested in developing predictable supramolecular chemistry using non-covalent urea-urea interactions to build functional materials.

Self-assembled bis-urea macrocycles: The study of enzymes has demonstrated that reactions carried out in confined environments proceed with extraordinary efficiency and selectivity. However, the development of synthetic reaction environments has been very challenging. We have identified bis-urea macrocyclic building blocks that predictably assemble to form porous crystalline materials (Figure 1). They are constructed from molecular units (bis-urea macrocycles) that are readily synthesized from rigid spacers and protected ureas. These macrocycles self-assemble one on top of each other by the urea hydrogen bonding motif and by aryl stacking to give functional materials that depend on the size of the macrocycle. Macrocycles that contain no cavity (Figure 1a) assemble to give strong pillars. Macrocycles with sizeable cavities (5-10 Å) assemble to give columns with accessible channels (Figure 1b). These columns subsequently pack together to form porous crystals with aligned one-dimensional channels. The dimensions of the homogeneous channels are controlled by the size of the macrocyclic units, which allows for precise and rational control over cavity dimensions, shape, and functionality. Strong pillars with external functional groups such as basic lone pairs (Figure 1c) afford materials that can expand like clays to accept guests in the flexible binding site in between the pillars. ***The goal of our research is to understand and apply this supramolecular assembly strategy to generate homogeneous microporous materials for use as confined environments for a wide range of chemical reactions.***

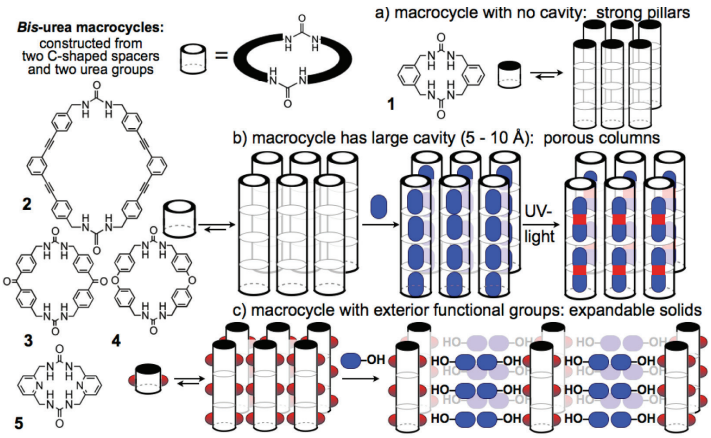

Fig. 1. The bis-urea macrocycle assembly motif. (a) Macrocycles that lack pores assemble into one-dimensional pillars. (b) Macrocycles that contain sizeable cavities give crystals with homogeneous channels (c) Macrocycles with exterior groups (red) may expand to absorb guests.

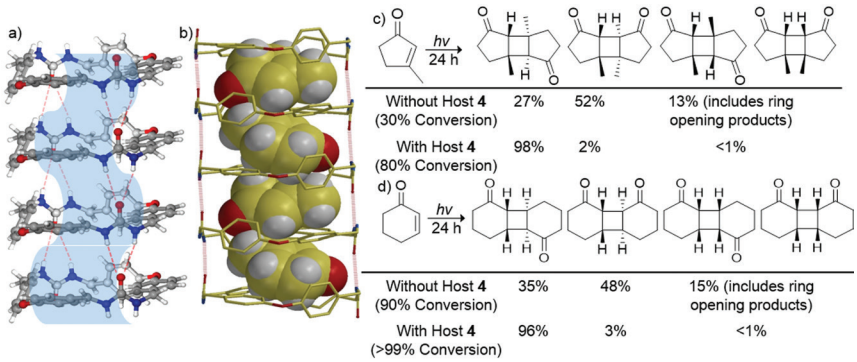

Fig. 2. Host 4 facilitates [2+2] cycloaddition of enones.

Reactions in confined environments. We are investigating the utility of functional porous to absorb, transport, and organize guests and to facilitate their subsequent photoreactions. Hosts **2**, **3**, and **4** show strong preferences for binding polar guests that are matched to the size and shape of the channels. These porous hosts are then used as 'stoichiometric' containers in the solid-state to facilitate reactions. This two-fold approach has several advantages. Characterization of the solid-state complexes allows us to probe how confinement in the channel influences the mechanism, product distribution, yield and selectivity for a specific reaction. Photoreactions and oxidations provide controlled model systems to test how effectively we can probe the effects of confinement on reactions. Ultimately, a better understanding of a reaction mechanism aids in the optimization of conditions and in the development of catalysts. For example, the zig-zag shaped channel (Figure 2) facilitates the [2+2]-cycloaddition of enone guests in high yield and high selectivity. We are probing the scope and application of these hosts as catalysts, and are investigating the use of host suspensions for mediating oxidations of alkenes by singlet oxygen in solution. Our goal is to expand to base-catalyzed reactions and polymerizations.

Representative Publications

Shimizu, L. S.; Salpage, S. R.; Korous, A. A. Functional Materials from self-assembled bis-urea macrocycles. *Acc. Chem. Res.* **2014**, ASAP article.

Xu, W. L.; Smith, M. D.; Krause, J. A.; Greytak, A. B.; Ma, S.; Read, C. M.; Shimizu, L. S. Single crystal to single crystal polymerization of a self-assembled diacetylene macrocycle. *Cryst. Growth Des.* **2014**, 14, 993-1002.

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Roy, K.; Wibowo, A. C.; Pellechia, P. J.; Ma, S.; Geer, M. F.; Shimizu, L. S. Absorption of hydrogen bond donors by pyridyl bis-urea crystals. *Chem. Mater.* **2012**, 24, 4773-4781.

NATALIA B. SHUSTOVA

ASSISTANT PROFESSOR

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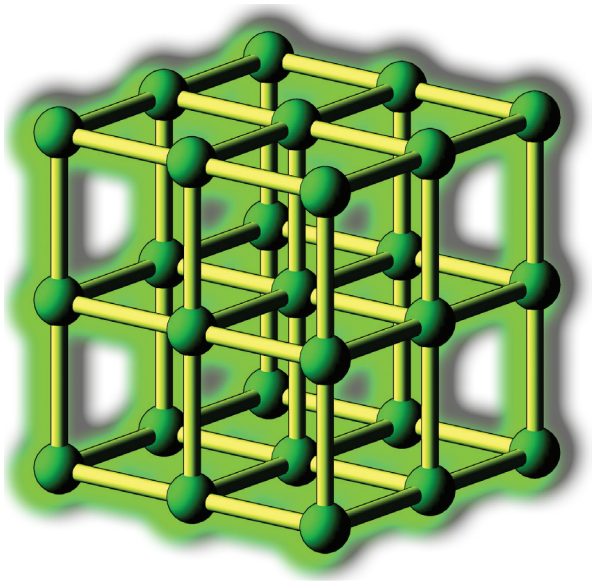
B.S., 2002 Moscow State University; M.S., 2004 Moscow State University; Ph.D., 2005, Physical Chemistry, Moscow State University; Ph.D., 2010, Inorganic Chemistry, Colorado State University; Postdoctoral Associate, 2012 Massachusetts Institute of Technology.

Research Areas: Inorganic and supramolecular chemistry, porous hybrid materials, switches, and crystallography.

Research in the group will be focused on materials for sustainable energy conversion, sensing, switches, and artificial biomimetic systems. Development of these materials will involve the synthesis and characterization of the porous (e.g., metal-organic frameworks (MOFs) and covalent-organic frameworks (COFs)) and graphitic materials. Specifically, three main directions related to 1) morphology control of the active layer of a bulk heterojunction solar cell, 2) light harvesting and energy transfer in well-defined self-assemblies, and 3) design of artificial scaffolds mimicking protein behavior will be developed.

Students who are interested in inorganic chemistry, materials, or physical chemistry are strongly encouraged to join. Each student in my group will be trained in synthesis and techniques for manipulating air-sensitive compounds, powder diffraction analysis, single-crystal X-ray crystallography, thermogravimetric analysis, and spectroscopy (UV-vis, IR, Fluorescence).



A concept of a hybrid luminescent material with controlled chromophore geometry, which is constructed out of metal nodes (green spheres) and organic linkers (yellow rods).

The Active Layer Morphology Control in Organic Photovoltaics. Increase of efficiency in the currently used bulk heterojunction solar cells, the realistic candidates for an efficient photoenergy conversion, can be achieved through the precise control of the active layer morphology at the nanoscale level. The ultimate goal of the research in my group is to design new materials that can be used as active layer components, which will lead to efficiency enhancement of solar cells.

Light Harvesting and Controllable Energy Transfer in Well-Defined Self-Assemblies. Light harvesting chromophore assemblies with an ability to control Förster resonance energy transfer (FRET) processes are required for the preparation of the next generation organic photovoltaics, molecular-scale digital switches, and sensors coupled to FRET. To address these issues, a new strategy to control energy transfer processes in self-assembled well-defined arrays of chromophores will be developed.

Representative Publications

Shustova, N. B.; Cozzolino, A. F.; Reineke, S.; Baldo, M.; Dincă, M. *J. Am. Chem. Soc.* **2013**, 135, 13326-13329.

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JAMES M. SODETZ

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B.A., 1970, Knox College; Ph.D., 1975, University of Notre Dame; NIH Postdoctoral Fellow, 1975–1977, Duke University Medical Center.

Established Investigator Award, American Heart Association, 1982–1987; Basic Science Research Award, University of South Carolina School of Medicine, 1990; Russell Research Award for Science, Mathematics, and Engineering, University of South Carolina, 2000; Carolina Trustee Professor Award, University of South Carolina, 2007; Elected Fellow, American Association for the Advancement of Science, 2010; South Carolina Governor's Award for Excellence in Scientific Research, 2011.

Research Areas: Biochemistry; protein chemistry, protein engineering, and molecular biology; structure-function studies of proteins and enzymes of blood with emphasis on the human complement system.

Our laboratory is studying the structure and function of a group of blood proteins which are components of the human "complement system." The complement system is composed of about 35 different proteins, enzymes, and regulatory molecules that interact to provide host defense against bacteria and other pathogenic organisms. One product of these interactions is C5b-9, a large protein complex composed of complement components C5b, C6, C7, C8 and C9. The C5b-9 complex is also referred to as the "membrane attack complex" (MAC) of complement because it forms a transmembrane pore on target cells. Formation of this pore disrupts membrane organization and contributes to bacterial cell killing. Assembly of the MAC is of biochemical interest because it occurs by a sequential, nonenzymatic mechanism and involves major hydrophilic to amphiphilic transitions by the constituent proteins. The binding interactions involved are complex and determined by distinct structural features on each protein. One goal of our lab is to identify those features.

Current efforts are focused on the physical and structural characterization of human C8 and analysis of its interaction with the other MAC components. Human C8 is an unusual protein composed of three nonidentical subunits referred to as α , β and γ. Through cDNA cloning and sequencing, we determined the complete amino acid sequence of C8 and gained valuable insight into how this protein functions. Specific roles for α and β have been identified and it appears that each subunit contains several different binding sites. We also determined that α, β and g are encoded in different genes. Genomic structures of α and β indicate these proteins share a close ancestral relationship to each other and to C6, C7 and C9. By contrast, γ is a member of the "lipocalin" family of proteins, and its role in the complement system is unknown.

Our study of human C8 utilizes the methods of modern biotechnology. All three subunits have been cloned and expressed as recombinant proteins in insect and mammalian cells. Truncated forms of α and β as well as full-length γ have also been produced in E. coli and used to investigate the location and properties of key binding sites. Several regions have been identified as being important in interactions with other components of the MAC, and with membrane proteins that regulate MAC activity. We also recently determined the X-ray crystal structure of human C8, a very large (150 kDa) protein. The structure suggest that human MAC proteins use a mechanism of pore formation that is similar to one used by bacterial pore-foming proteins, i.e. the cytolysins. By further exploring these and other structure-function relationships within the MAC proteins we hope to gain a better understanding of MAC formation and function. Such information will be useful for developing inhibitors of the MAC and for engineering MAC analogues that could destroy undesirable cells, e.g. tumor cells.

Representative Publications

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Scibek, J. J.; Plumb, M. E.; Sodetz, J. M. Binding of Human Complement C8 to C9: Role of the N-Terminal Modules in the C8α Subunit. *Biochemistry* **2002**, 41, 14546-14551.

Parker, C. L.; Sodetz, J. M. Role of the Human C8 Subunits in Complement-Mediated Bacterial Killing: Evidence that C8γ is not Essential. *Mol. Immunol.* **2002**, 39, 453-458.

Musingarimi, P.; Sodetz, J. M. Interaction between the C8α-γ and C8b Subunits of Human Complement C8: Role of the C8β N-Terminal Thrombospondin Type 1 Module and Membrane Attack Complex/Perforin Domain. *Biochemistry* **2002**, 41,11255-11260.

Ortlund, E.; Parker, C. L.; Schreck, S. F.; Ginell, S.; Minor, W.; Sodetz, J. M.; Lebioda, L. Crystal Structure of Human Complement Protein C8γ α1.2Å Resolution Reveals a Lipocalin Fold and a Distinct Ligand Binding Site. *Biochemistry* **2002**, 41, 7030-7037.

Plumb, M. E.; Sodetz, J. M. An Indel Within the C8α Subunit of Human Complement C8 Mediates Intracellular Binding of C8γ and Formation of C8α-γ. *Biochemistry* **2000**, 39, 13078-13083.

MORGAN STEFIK

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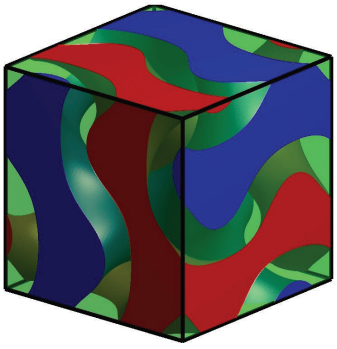
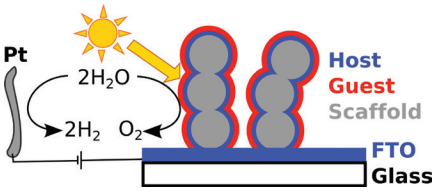
Research Areas: Functional nanostructures, alternative energy devices, block copolymers, self-assembly, nanoparticles, photonics, atomic layer deposition, (photo)electrochemistry.

The Stefik group is developing new polymer derived nanomaterials and alternative energy devices. We are interested in bottom-up methods based upon the self-assembly of either polymers, nanoparticles, or mixtures thereof to form complex materials with nanoscale control. Such nanomaterials are critical for developing numerous technologies that rely upon tunable electronic, optical, or catalytic characteristics, for example. Many of our projects focus on alternative energy applications such as fuel cells, batteries, supercapacitors, photovoltaics, and solar fuels. Our focus on bottom-up methods makes our discoveries easily deployable to industry for a significant and real impact.



Self-Assembly: Block copolymers are a fascinating class of molecules that can self-assemble into a diverse range of structures. They can be thought of as separate homopolymers, for example A and B, that have been connected to each other via a bond. Generally, the enthalpic penalty for A-B contacts dominates the free-energy and drives the blocks to phase separate from each other on the 1-100 nm length scale. The resulting nanostructures have precisely defined pathways and interfaces that have yet to be fully applied towards nanoscale devices. A powerful feature of self-assembly is that access to such tailored nanomaterials is possible with affordable beaker chemistry, enabling direct translation to affordable mass production. One of our goals is to develop the new materials chemistry needed to self-assemble the diverse range of nanomaterials needed for advanced technologies and devices.

(Photo)electrochemistry: The limited fossil fuel supplies coupled with environmental concerns motivate our quest for improved sustainable energy sources. Key energy technologies, including photovoltaics, batteries, supercapacitors, fuel cells, and solar fuels all rely upon electrochemistry with reactions occurring at controlled interfaces and multiple species migrating along continuous pathways. Here, materials with sufficient power for practical devices require fast reaction rates and thus rely upon nanostructured materials having lots of active interfacial area. Thus developing techniques to organize and arrange multiple functional materials on the nanoscale is critical to advancing many (photo)electrochemical platforms for alternative energy.



Atomic Layer Deposition: ALD is a remarkable technique for building nanoscale devices. A series of exposures to chemical vapors is used to deposit atomically-thin material layers in a conformal fashion based upon a cycle of self-limiting surface-reactions. A powerful and unique feature of ALD is that it can deposit into pores of high surface area materials to build multiple-layers of functional materials for nanoscale devices. Such strategies can be used to decouple electronic transport from, for example, optical or diffusional constraints enabling new high performance devices.

Skills and Techniques: The focus of our lab is the synthesis and characterization of nanomaterials as well as their application to advanced devices. Thus, materials chemistry is at the heart of much of our work with particular attention to polymer and inorganic chemistry. For this we use air-free synthesis techniques including Schlenk lines and gloveboxes for polymer and nanoparticle synthesis. These base materials are characterized with NMR, GPC, and electron microscopy. After self-assembly, nanostructures are characterized by additional electron microscopy techniques, including 3D tomographic reconstructions, XRD, Raman, TGA, BET, and small-angle x-ray scattering. Additional levels of complexity are added by post modification with for example atomic layer deposition and the final (photo)electrochemical devices are analyzed with 2/3-electrode potentiostats and electrochemical impedance spectroscopy.

Representative Publications

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Hisatomi, T.; Dotan, H.; Stefik, M.; Sivula, K.; Rothschild, A.; Grätzel, M.; Mathews, N., Enhancement in the performance of ultrathin hematite photoanode for water splitting by an oxide underlayer. *Adv. Mater.* **2012**, 24 (20), 2699-2702.

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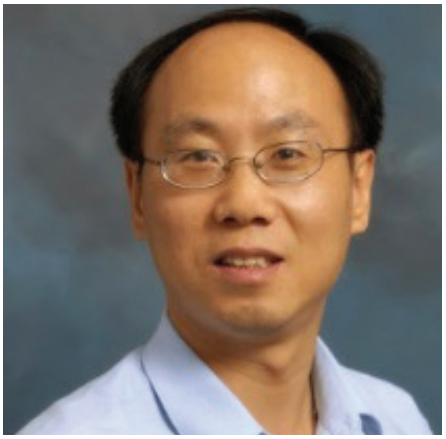

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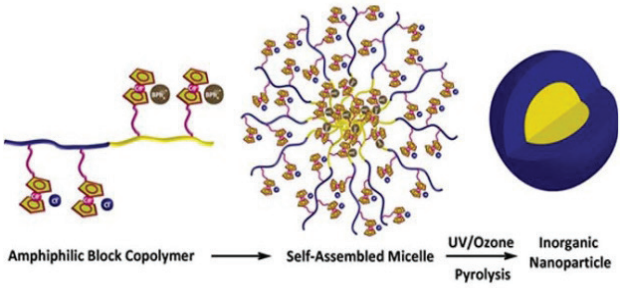

Figure 2. Self-assembly of cobaltocenium-containing block copolymers and synthesis of inorganic nanoparticles.

B.S., 1997, Nanjing University; Ph.D., 2006, Carnegie Mellon University; Postdoctoral Fellow, 2006–2009, University of California at Santa Barbara.

Singapore National Research Foundation Research Fellow, 2009; Academy of Forestry, Visiting Professor, since 2009; Doctoral New Investigator Award, ACS PRF 2012; ACS Leadership Development Award Alternate, 2013; ACS Committee on Project Seed, 2012-2015; NSF CAREER Award, 2013; ACS Polymeric Materials: Science and Engineering (PMSE) Young Investigator, 2014;

Research Areas: Organic polymer synthesis. controlled/living polymerization, renewable polymers from biomass, organometallic polymers, antimicrobials, polymer nanodielectric materials, macromolecular self-assembly, polymers for biomedical applications.

Renewable Polymers from Biomass: Synthesis of renewable polymeric materials from natural resources has become a rapidly growing area as these materials could replace environmentally and energy unfavorable plastics derived from petroleum chemicals. We have developed a variety of renewable monomers and polymers using hydrocarbon-rich natural resource. Our goal is to revolutionize traditional renewable polymers and develop new classes of green polymers such as thermoplastic elastomers, degradable polymers, stimuli-responsive polymers and natural fiber reinforced nanocomposites.

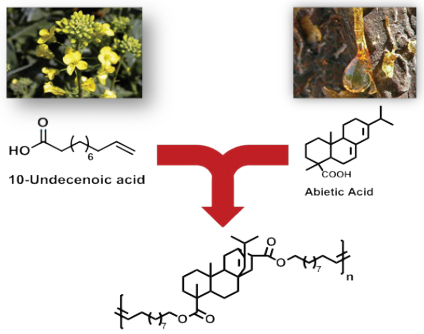

Figure 1. Renewable bio-based polymers

Metallocene Polymers: Metallocene containing polymers have attracted significant attentions since they have great potentials in catalytic, optical, magnetic, and biological applications as well as uses for semiconductors, lithographic resists, and ceramic precursors. We have developed a broad spectrum of novel metallocene monomers. The goal is to explore a wide range of metallocene polymers and to lay out synthetic foundation of this type of polymers for many potential applications.

Antimicrobial Polymers: In recent years, considerable research has been focused on developing synthetic antimicrobial agents that could mimic antimicrobial peptides or replace expensive synthetic peptides. We discover that natural resin acid-derived cationic compounds and polymers exhibit high antimicrobial activities against a broad spectrum of bacteria without inducing hemolysis of red blood cells. We aim to design various macromolecular architectures to tune the antimicrobial activity of cationic polyelectrolytes and utilizing them for biomedical applications such as antibiotics and medical device coatings.

Polymer Nanodielectric Materials: There is much demand for the development of pulse power, which requires accumulating much energy over a relatively long period of time and releasing it quickly thus increasing the instantaneous power. We use certain organic pi-conjugated systems, such as oligoaniline, oligothiophene, etc., dispersed in an insulating polymeric matrix to form nano-dipolar domains, which would allow fast polarizability response under high frequency electric fields. Our goal is to develop interfacially-dominated polymeric materials based on nanophase-separated homopolymers and block copolymers that store energy via electronic conduction and interfacial polarization.

Macromolecular Self Assembly: The self-assembly of block copolymers in thin films has drawn much attention due to its potential applications in microelectronic devices, data storage system, membranes, etc. Solution self-assembly allows for block copolymers to self-assemble into various morphologies including micelles, vesicles, rods, and tubes. These nanostructures have numerous applications such as drug delivery, templates toward ordered metallic, magnetic, and inorganic nanoobjects. By investigating new strategies, we aim to combine novel block copolymer chemistries with long-range ordering to further develop block copolymer self-assembly to target various applications.

Representative Publications

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Zheng, Y.; Yao, K.; Lee, J.S.; Chandler, D.; Wang, J.; Wang, C.; Chu, F.; Tang, C. Well-defined polymers derived from gum rosin. *Macromolecules* **2010**, 43, 5922–5924.

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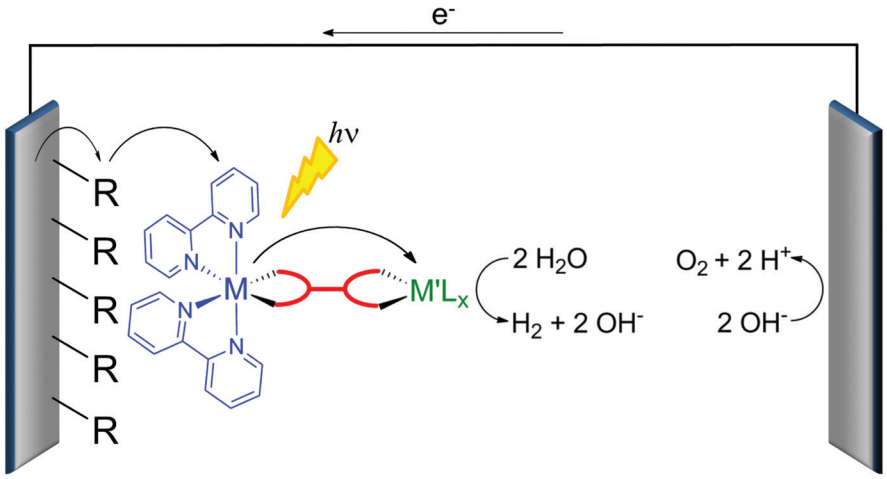

Figure 1. Schematic for H_2 production from water splitting, utilizing modified electrodes for the necessary reductive quenching step.

Research Areas: Inorganic chemistry; electrochemistry; catalysis; organometallics; renewable energy; design, synthesis, and characterization of transition metal catalysts capable of small molecule transformations.

Furthering alternative energy research is of upmost importance as the negative effects of man-made carbon emissions are becoming much clearer. Modern energy challenges involve the catalytic transformation of inert small molecules through redox events. Electrochemical methods will play a large role in discovering and further developing catalysts capable of these transformations.

Light Driven Fuel Production: Efficient conversion of light-to-chemical energy provides an attractive approach to the development of alternative energy sources. The production of fuels from a renewable, carbon neutral source and sunlight is an important technological goal for energy research and sustainability. Targets include production of H_2 from water splitting, and light hydrocarbons from the reduction of carbon dioxide. The development of intramolecular chromophore-catalyst assemblies capable of efficient charge separation is essential to this project. The design of the chromophore catalyst assemblies focuses on combining the individual components – chromophore, bridging ligand, and catalyst – with the proper energy levels to promote electron transfer from the chromophore to the catalyst. In addition, one major disadvantage of current photocatalytic systems is the requirement for chemical sacrificial electron donors (SEDs) for reductive quenching of the chromophores. An ideal alternative to SEDs is utilizing high surface area electrodes. Applying a small voltage bias to conductive electrodes – glassy carbon, Pt, Au – chemically modified with diodes should be a viable reductive quenching route.

Cross Coupling: Routes to Higher Hydrocarbons: Carbon-carbon cross coupling is arguably the most important class of organic reactions, but is still limited with respect to coupling molecules containing β-hydrogen atoms. Conventional cross coupling between carbon nucleophiles and carbon electrophiles can suffer from oxygen sensitivity, kinetically slow transmetalation steps, air and moister sensitivity of the carbon nucleophiles compared to analogous carbon electrophiles, and solubility and compatibility problems from a wide mixture of chemicals required for the coupling reactions. Conversely, electrochemical cross coupling offers a wider range of cross coupling partners, removes the need for many chemical additives to activate the reactions, and removes the kinetically limiting transmetalation step. A major thrust is to expand the applicability and range of electrochemically driven reductive cross coupling with a focus on furthering cross coupling reactions beyond the limitations of currently utilized routes. Developing electrochemical reductive cross coupling chemistry with kinetically facile routes for C–C coupling products offers a mechanistic scheme to prevent unwanted β-hydride elimination products, which could lead to the low temperature production of liquid hydrocarbon fuel from abundant light hydrocarbons. In addition, the reductive C-C coupling scheme is ideal for incorporating catalytic carboxylation reactions using carbon dioxide as an inexpensive and completely renewable chemical feedstock. The utilization of CO_2 for the production of fuels, polymers, and synthetic precursors could also help mitigate current CO_2 emission problems.

Representative Publications

Vannucci, A. K.; Alibabaei, L.; Losego, M. D.; Concepcion, J. J.; Berç, K.; Parsons, G. N.; Meyer, T. J. Crossing the Divide between Homogeneous and Heterogeneous Catalysis. *Proc. Natl. Acad. Sci.* **2013,** 110, 20918.

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THOMAS VOGT

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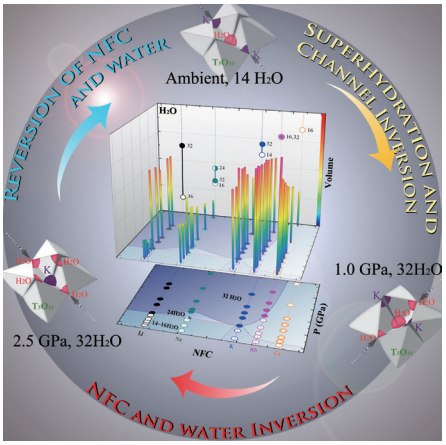
Diplom, 1985, University of Tübingen University of Tübingen, Germany; Ph.D., 1987, University of Tübingen, Germany

Scientist, 1988–1992, Institute Laue-Langevin, Grenoble, France; Physicist, 1992–2000, Brookhaven National Laboratory (BNL); Group Leader Powder Diffraction, 2000–2003, BNL; Head of Materials Synthesis & Characterization Group, 2003–2005, BNL; fellow of the American Physical Society, 2006; fellow of the American Association for the Advancement of Science, 2008; International Visiting Research Fellowship at the University of Sydney, Australia, 2009; adjunct faculty at the African University of Science and Technology in Abuja, Nigeria, 2009.

Research Areas: Crystallography; general structural chemistry; chemical synthesis, structures, and properties of metal oxides; electron, x-ray, and neutron diffraction techniques and instrumentation (i.e high pressure x-ray diffraction, high-temperature electron microscopy)

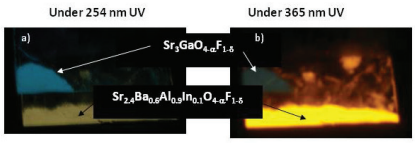
Research Project 1: Pressure-Induced Hydration and Insertion of CO_2, noble gases and rare earth metal cations.



Supported by a Global research Laboratory of the Korean Ministry of Education, Science and Technology we have been studying the Insertion of water, CO_2 , rare earth metal cations and noble gases in the small pore zeolite natrolite.

Research Project 2: New Phosphors for Up- and Down-Conversion of Light

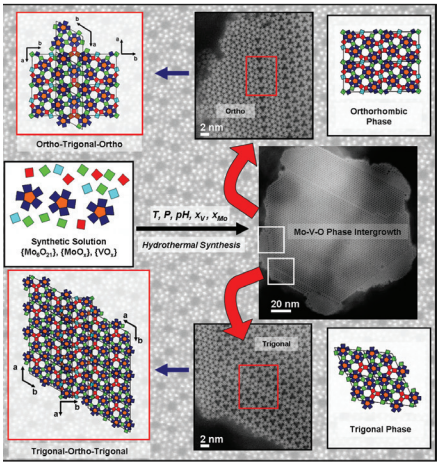
Luminescenece, the absorption of energy with subsequent emission of light and, more specifically, fluorescence, the absorption of energy with subsequent emission of light in the visible spectrum, are the basis of a broad range of everyday applications such as lighting and x-ray detectors for medical and technical applications. Luminescent materials, also called phosphors, consist of a host lattice in which activator ions are doped into in small concentrations, typically less than a mole percent. The activator ions have energy levels that can be populated by direct excitation or indirectly by energy transfer and are responsible for the luminescence. We have discovered a new family of luminescent materials and are currently exploring its use in white light LED applications as well as upconversion applications such as biomedical imaging. This work involves solid-state synthesis, structural characterization using x-ray powder diffraction, and extensive characterization of the optical properties.



Research Project 3: Imaging at the Nanoscale.

High-Angle-Annular-Dark-Field/Scanning Transmission Electron Microscopy (HAADF/STEM) is a technique uniquely suited for detailed studies of the structure and composition of complex oxides. The HAADF detector collects electrons that interact inelastically with the potentials of the atoms in the specimen and therefore resembles the better known Z^2 (Z is atomic number) Rutherford scattering. One class of important catalysts consists of bronzes based on pentagonal $\{Mo_6O_{21}\}$ building units; these include Mo_5O_{14} and $Mo_{17}O_{47}$. In the last 20 years, new materials doped with a variety of substitution elements, but built upon the same structural building units, have been made and evaluated for their catalytic properties. Applications include the selective oxidation of light paraffins and olefins, as well as the partial oxidation of methanol.

We engage in HAADF-STEM investigations of various complex oxide phases and have shown that we can, for example, distinguish metal-containing sites within these structurally and compositionally complex-oxides through Z^2-contrast analysis. We compare our experiments to image simulations that are done in collaboration with the Interdisciplinary Mathematics Institute here at USC. Collaboration with Douglas Blom (University of South Carolina) and Douglas Buttrey (University of Delaware).



REPRESENTATIVE PUBLICATIONS

Lee,Y.; Lee, Y.; Seoung, D.; Im, J-H.; Hwang, H-J.; Kim, T-H.; Dan Liu, Liu, Z.; Lee, S.Y.; Kao, C-C. Thomas Vogt, T. Immobilization of Large, Aliovalent Cations in the Small Pore Zeolite K-Natrolite using Pressure. *Angew. Chem. Intl. Ed.* **2012**, 51(20), 4848-4851.

Lee, Y.; Seoung, D.; Jang, Y-N.; Vogt, T.; Lee, Y. Pressure-Induced Hydration and Insertion of CO2 in Ag-Natrolite.*Chem- Eur. J.* **2013**, 19, 5806-5811.

Lee, Y.; Seoung, D.; Lee, Y.; Kao, C-C.; Vogt, T. Super-Hydrated Zeolites: Pressure-Induced Hydration in Natrolites. *Accepted Chem. – Eu. J.* **2013.**

Pyrz, W.D.; Blom, D.A.; Buttrey, D.J.; Vogt, T. High-Angle Annular Dark field Scanning Transmission Electron Microscopy (HAADF-STEM) Investigations of Bimetallic nickel-Bismuth Nanomaterials Created by Electron Induced Electron Beam Induced Fragmentation (EBIF). *J. Phys. Chem. C* **2010**, 114, 2538–2543.

Pyrz, W.D.; Blom, D.A.; Sadakane, M.; Kodato, K.; Ueda, W.; Vogt, T.; Buttrey, D.J. Atomic-Level Imaging of Mo-V-O Complex Oxide Phase Intergrowth, Grain Boundaries, and Defects using HAADF-STEM. *Proc. Natl. Acad. Sci.* **2010**, 107 (14), 6152–6157.

Pyrz, W.D.; Blom, D.A.; Sadakane, M.; Kodato, K.; Ueda, W.; Vogt, T. ; Buttrey, D.A. Atomic-Scale Investigation of Two-Component MoVO Complex Oxide Catalysts Using Aberration-Corrected High-Angle Annular Dark-Field Imaging. *Chem. Mater.* **2010**, 22 (6), 2033–2040.

Park, S., Vogt, T. Near UV Excited Line and Broad Band Photoluminescence of an Anion-Ordered Oxyfluoride. *J. Am. Chem. Soc.* **2010**, 132, 4516.

Pyrz, W.D., Blom, D.A.; Vogt, T.; Buttrey, D.J. Direct Imaging of the MoVTeNbO M1 Phase using a Cs-corrected High-resolution Scanning Transmission Electron Microscope (STEM). *Angew. Chem. Int. Ed.* **2008**, 47, 2788–2791.

HUI WANG

ASSISTANT PROFESSOR

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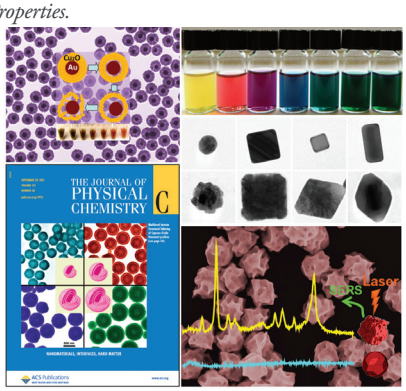
B.S., 2001, Nanjing University; Ph.D., 2007, Rice University (Advisor: Naomi J. Halas); Postdoctoral fellow, 2007–2010, University of Texas at Austin (Advisor: Paul F. Barbara).

Honors and Awards: NSF CAREER Award, 2013; USC Breakthrough Star Award, 2014.

Research Areas: Nanoscience; Surface-enhanced spectroscopy; Biophysics; Bioanalytical chemistry

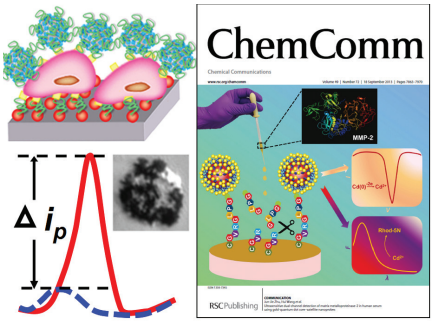
The central theme of our research is to use physical chemistry approaches, specifically spectroscopy and electrochemistry, to tackle challenging problems in materials and biological sciences.

Nanostructures with Geometrically Tunable Optical Properties.



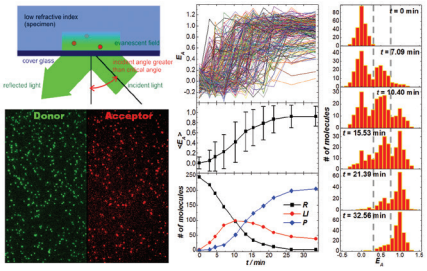
Nanophotonic materials have emerged as an important class of subwavelength optical components that interact with light in unique ways on the nanometer length-scale. Our interests in nanophotonic materials broadly span several important aspects in this field, including but not limited to nanostructure fabrication, nanoscale self-assembly, structure-property relationship, and applications of these materials. We have been working on several nanostructures with geometrically tunable optical properties, such as semiconductor nanoshells, metal-semiconductor core-shell heteronanostructures, and complex metallic nanoparticles. We are particularly interested in (i) development of new approaches for the controllable fabrication of optically active nanostructures; (ii) utilization of optically active nanostructures as building blocks to assemble mesoscopic structures over multiple length scales; (iii) detailed characterization of the optical properties of these nanomaterials both at the ensemble and single-nanoparticle levels; (iv) development of quantitative understanding on the structure-property relationship of these nanostructures through combined experimental and theoretical efforts; and (v) applications of these nanophotonic materials in surface-enhanced spectroscopies for ultrasensitive molecular sensing.

Multifunctional Nanoprobes for Electrochemical Cytosensing.



The past two decades have witnessed significant progress on the development of robust analytical tools with high sensitivity, selectivity, and reproducibility toward early diagnosis of cancer. Electrochemical cytosensing has emerged as an extremely attractive method that can be readily implemented into quantitative bioassays for high-throughput clinical applications. Utilization of rationally designed multifunctional nanoprobes and specifically tailored nano-biointerfaces for electrochemical cytosensing provides unique opportunities to optimize the interfacial electron transfer and cell recognition processes, allowing for the integration of large signal amplification, enhanced detection specificity, and expanded multiplex sensing capabilities on one cytosensor. Our group has been working on the design and fabrication of multifunctional hybrid nanoprobes for selective and ultrasensitive electrochemical detection of a variety of cancer cells, such as leukemia cells and circulating tumor cells. Our electrochemical approaches also allow for the quantification of the expression levels of important biomarkers on the cancer cell surfaces.

Single-Molecule Biophysics. Our group has been working on the development of detailed, molecular-level understanding of important nucleic acid (NA)



structural remodeling processes chaperoned by retroviral nucleocapsid (NC) proteins. In spite of their structural simplicity, retroviral NC proteins exhibit a diverse set of biological functions that are crucial to the retroviral life-cycles. The role of NC proteins as NA chaperones is perhaps their most important function ever known so far. NC proteins promote several NA structural remodeling processes that are crucial to the retroviral life-cycles, such as the obligatory strand transfers in the reverse transcription, the maintenance and integration of proviral DNA, and the genomic RNA protection and packaging. NC-chaperoned NA structural remodeling typically involves various intermediates along multiple reaction pathways and is tightly associated with heterogeneous conformational dynamics over multiple time-scales that cannot be synchronized and resolved by ensemble measurements. Single-molecule spectroscopy provides an extremely powerful way to characterize such complex biomolecular processes without the ensemble averaging effects. Our group uses time-resolved single-molecule spectroscopy as an analytical tool to study the kinetics and mechanism of NC-chaperoned NA annealing that occurs during the reverse transcription and to resolve the conformational dynamics associated with NC-induced local bending of proviral DNA. These single-molecule measurements allow us to gain molecular-level insights on the complicated, dynamic NC-NA interactions that underpin NCs' NA chaperone functions.

Representative Publications

Zheng, T.; Zhang, Q.; Feng, S.; Zhu*, J. J.; Wang, Q.; Wang, H.* Robust Nonenzymatic Hybrid Nanoelectrocatalysts for Signal Amplification toward Ultrasensitive Electrochemical Cytosensing. *J. Am. Chem. Soc.* **2014**, 136, 2288-2291.

Zhang, Q.; Large, N.; Nordlander, P.; Wang, H.* Porous Au Nanoparticles with Tunable Plasmon Resonances and Intense Field Enhancements for Single-Particle SERS. *J. Phys. Chem. Lett.* **2014**, 5, 370-374.

Zheng, T.; Zhang, R.; Zhang, Q.; Tan, T.; Zhang, K.; Zhu, J. J.*; Wang, H.* Ultrasensitive Dual-Channel Detection of Matrix Metalloproteinase-2 in Human Serum Using Gold-Quantum Dot Core-Satellite Nanoprobes. *Chem. Comm.* **2013**, 49, 7881-7883.

Zhang, L.; Jing, H.; Boisvert, G.; He, J. Z.; Wang, H.* Geometry Control and Optical Tunability of Metal-Cuprous Oxide Core-Shell Nanoparticles. *ACS Nano* **2012**, 6, 3514–3527.

Zhang, L.; Wang, H.* Cuprous Oxide Nanoshells with Geometrically Tunable Optical Properties. *ACS Nano* **2011**, 5, 3257-3267.

QIAN WANG

CAROLINA DISTINGUISHED PROFESSOR

wang263@mailbox.sc.edu

B.A., 1992, Tsinghua University, China; Ph.D., 1997, Tsinghua University, China; Postdoctoral Fellow, 1997–1999, University of Lausanne; Skaggs Postdoctoral Fellow, 1999–2001, and Senior Research Associate, 2003, The Scripps Research Institute.

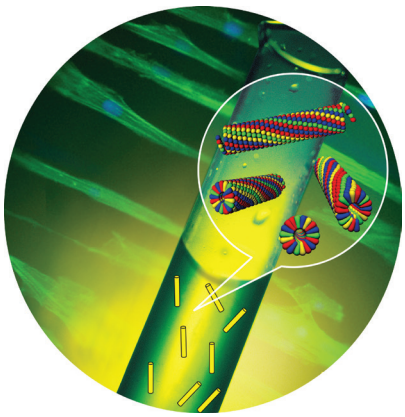
National Science Foundation CAREER Award, 2008; Alfred P. Sloan Foundation Research Fellow, 2008; Camille Dreyfus Teacher-Scholar Award, 2008; CAPA Distinguished Junior Faculty Award, 2008; South Carolina Governor's Young Researcher Award for Excellence in Scientific Research, 2009; USC Breakthrough Rising Star, 2010; AAAS Fellow, 2012.

Research Areas: Organic synthesis, bioconjugation chemistry, biomaterials chemistry, and soft materials.

Introduction: The central concept of our research is how to marry organic chemistry with the logic of biology in order to develop new materials and solve the problems in chemistry and biology. Synthetic chemistry and molecular biology will be employed as the major tools to pursue our research. Students will work in a highly interdisciplinary research team and will have the opportunity to learn a variety of techniques, such as organic synthesis, combinatorial chemistry, molecular biology, and modern instrumental analysis. Some of the areas that we are interested in are as follows:

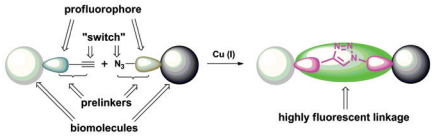
Bionanoparticles as molecular scaffolds: Bionanoparticles (BNPs), including viruses, ferritins, and self-assembled protein cages, can be considered building blocks, scaffolds, and nanoreactors for chemical operations and materials development. Many BNPs are structurally well characterized at near atomic resolution and can be safely handled and easily obtained in large quantities. BNPs can be treated as "*molecules*" by synthetic chemists. Each BNP has unique physical, chemical, and biological properties. Despite viruses' greater structural and functional complexities in comparison to other biomolecules such as nucleic acids and proteins, the shell proteins of BNPs are well-arrayed as helical or spherical morphology. These features make BNPs very attractive polyvalent platforms for developing new chemistry and materials (Figure). We will exploit non-enveloped icosahedral or helical viruses and ferritins as scaffolds in chemical reactions. Upon chemical or genetic modification, various functionalities (i.e. sensing moieties, enzyme mimetic sites, energy harvesting molecules, cell targeting and permeating groups, in vivo imaging reagents, and DNA binding groups, etc.) will be engineered on the exterior or the interior surface, to create novel functional nanoparticles. In addition, the viral shell proteins (capsids) constrain a special microenvironment that will be employed as a "nano-vessel" for chemical reactions.

Developing new biomaterials on the basis of self-assembly. Quantitative understanding of the chemical, physical, dynamic, and mechanical aspects of nanoparticle-based self-assembly to form hierarchically ordered structures at the nanometer scale is the basis of novel



optical, acoustic, electronic, and magnetic materials and devices. A fundamental disadvantage in the use of synthetic nanoparticles for such studies is the inherent polydispersity of the particle size and non-uniformity of their surface properties. In addition, the chemistries associated with particle fabrication are difficult, and the degree of functionality of the particles is always uncertain. In contrast, BNPs are monodisperse in size and can be functionalized in a robust, well-defined manner under the control of malleable genetic information. These properties, unique to BNP's, make them uniquely suited for studies of self-assembly that will have broad applications. Our major efforts will focus on two aspects: interfacial assembly of BNPs between immiscible fluids (Figure) and hierarchical self-assembly of BNPs with diblocks copolymers. By the chemical and genetic modification on the basis of the structure information, we hope to program the viral particle to form controllable one-, two-, or three-dimensional arrays.

Fluorogenic reactions for bioconjugation and bioimaging: We have developed a series of fluorogenic CuAAC reactions. In addition to being used in the combinatorial synthesis of fluorescent dyes, the most important application of these reactions is the bioconjugation



and bioimaging within the intracellular environment. Incorporation of exogenous natural or unnatural tags into proteins or glycans by cellular biosynthetic pathways is an emerging strategy for investigating their cellular activities. Since those processes involve multistep enzymatic transformations that prohibit the incorporation of large signaling moieties, chemoselective reactions are often employed for post-labeling. In this case, a bioorthogonal fluorogenic reaction is invaluable, in which unreacted reagents show no fluorescent background and the purification process can be circumvented. One of the 3-azidocoumarins developed in our group had been successfully utilized for in vivo protein labeling studies.

Representative Publications

Li, T.; Zan, X.; Winans, R. E.; Wang, Q.; Lee, B. Biomolecular assembly of thermoresponsive superlattices of the tobacco mosaic virus with large tunable interparticle distances. *Angew. Chem. Int. Ed.* **2013**, 52, 6638-6642.

Zan, X.; Feng, S.; Balizan, E.; Lin, Y.; Wang, Q. General and facile method to align one dimensional nanoparticles in macro scale and control over myoblast orientation and differentiation. *ACS Nano* **2013**, 7, 8385-8396. (Highlighted as the front cover)

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Liu, Z.; Qiao, J.; Niu, Z.; Wang, Q. Natural supramolecular building blocks: from virus coat proteins to viral nanoparticles. *Chem. Soc. Rev.* **2012**, 41, 6178–6194.

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Le Droumaguet, C.; Wang, C.; Wang, Q. Fluorogenic Click Reaction. *Chem. Soc. Rev.* **2010**, 39, 1233–1239 (cover paper).

Kaur, G.; Valarmathi, M.T.; Potts, J.D.; Jabbari, E.; Sabo-Attwood, T.; Wang, Q. Regulation of osteogenic differentiation of rat bone marrow stromal cells on 2D nanorod substrates. *Biomaterials* **2010**, 31, 1732–1741.

Lin, Y.; Balizan, E.; Lee, L.A.; Niu, Z.; Wang, Q. Self-assembly of rod-likebionanoparticles in capillary tube. *Angew. Chem. Int. Ed.* **2010**, 49, 868–872.

SHERYL WISKUR

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B.S., 1997, Arizona State University; Ph.D., 2003, University of Texas–Austin; Postdoctoral Associate, Massachusetts Institute of Technology, 2003–2005.

NSF CAREER Award 2011-2016; SC EPSCoR Diversity Award 2012; USC Breakthrough Rising Star, 2013.

Research Areas: Synthetic methodology, organocatalysis, physical organic, bioorganic, sensors

My research interests lie within the area of synthetic organic methodology. We are focused on developing facile methods to efficiently resolve and isolate medicinally important enantiopure compounds. Most recently we have been focused on kinetic resolutions toward accomplishing this goal, and exploring the mechanism of the methodology we have developed.

Optically active intermediates are of increasing importance in the pharmaceutical and agrochemical industries as the number of active chiral compounds in their pipelines grow. Chiral alcohols and amines are of particular importance in the development of many products for these industries. While there are ways to form these compounds asymmetrically, industry has still found kinetic resolutions to be a very efficient and economical way to obtain enantiomerically pure compounds. A kinetic resolution is a separation of enantiomers by selectively reacting one enantiomer over the other in an asymmetric reaction. This works when one of the enantiomers reacts faster than the other (kS > kR). Kinetic resolutions are evaluated by selectivity factors, which is a ratio of the rate of the fast reacting enantiomer over the rate of the slow reacting enantiomer (Figure 1). One of the advantages of a kinetic resolution over an asymmetric reaction is

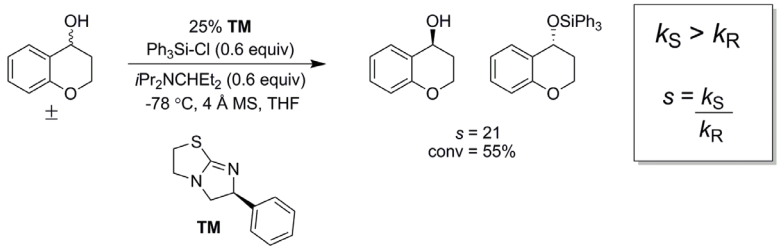

Figure 1. The kinetic resolution of chromanol by selectively silylating one enantiomer and leaving the other one alone. Kinetic resolutions are evaluated by a ratio of the rates of the two enantiomers.

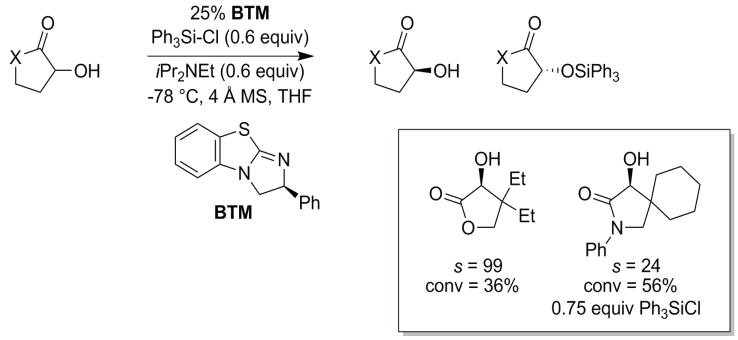

Figure 2. Silylation-based kinetic resolution of α-hydroxy lactones and lactams. Selectivities close to 100 were observed.

that the enantiomeric excess of the starting material is continuously increasing as the reaction progresses. This allows for the recovery of highly enriched material, even when the resolution only has moderate selectivity.

We have developed new strategies for the separation of alcohols. Our approach towards this employs a silyl group to asymmetrically derivatize one enantiomer over another. We have employed this to resolve cyclic secondary alcohols such as chromanol (Figure 1) and α-hydroxy lactones and lactams (Figure 2). These compounds are all important starting materials in the synthesis of biologically active compounds.

In order to further improve our reaction, an understanding of the mechanism is crucial. We have employed different physical organic techniques in order to gain some understanding of the mechanism, including a linear free energy relationship study and a kinetic study. The ultimate goal is to determine how all the pieces come together to asymmetrically silylate one enantiomer, yet not silylate the other one. This information will help us continue to expand our methodology to include other substrates and other classes of compounds.

Representative Publications

Akhani, R. K.; Moore, M. I.; Pribyl, J. G.; Wiskur, S. L. Linear Free-Energy Relationship and Rate Study on a Silylation-Based Kinetic Resolution: Mechanistic Insights. *J. Org. Chem.* **2014**, *79*, 2384-2396.

Clark, R. W.; Deaton, T. M.; Zhang, Y.; Moore, M. I.; Wiskur, S. L. Silylation-Based Kinetic Resolution of α-Hydroxy Lactones and Lactams. *Org. Lett.* **2013**, *15*, 6132-6135.

Nguyen, D.; Akhani, R. K.; Sheppard, C. I.; Wiskur, S. L. A Structure-Activity Relationship of Formamides as Organocatalysts: The Significance of Formamide Structure and Conformation. *Eur. J. Org. Chem.* **2013**, 2279–2283.

Wiskur,S. L.; Maynor, M. S.; Smith, M. D.; Sheppard, C. I.; Akhani, R. K.; Pellechia, P. J.; Vaughn, S. A.; Shieh, C. Chiral pyridinyloxazolidine ligands and copper chloride complexes. *J. Coord. Chem.* **2013**, *66*, 1166-1177.

Klauck, M; Patel, S. G.; Wiskur, S. L. Obtaining Enriched Compounds via a Tandem Enantioselective Reaction and Kinetic Resolution Polishing Sequence. *J. Org. Chem.* **2012**, *77*, 3570-3575.

Sheppard, C. I.; Taylor, J. L.; Wiskur, S. L. Silylation-Based Kinetic Resolution of Monofunctional Secondary Alcohols. *Org. Lett.* **2011**, *13*, 3794–3797.

Patel, S. G.; Wiskur, S. L. Mechanistic Investigations of the Mukaiyama Aldol Reaction as a Two Part Enantioselective Reaction. *Tetrahedron Lett.* **2009**, *50*, 1164-1166.

HANS-CONRAD ZUR LOYE

ASSOCIATE DEAN FOR RESEARCH; DAVID W. ROBINSON PALMETTO PROFESSOR
zurloye@mailbox.sc.edu

Sc.B., 1983, Brown University; Ph.D., 1988, University of California at Berkeley; Postdoctoral, Fellow 1988–1989, Northwestern University.

Camille and Henry Dreyfus New Faculty Award, 1989; Exxon Award in Solid State Chemistry, 1994; Guest Professor Shandong Normal University, 2001; Visiting Professor at the ICMCB-CNRS-Bordeaux, France, 2003; Visiting Professor Sun Yat-sen University, 2008; IPMI Henry J. Albert Award, 2009; Elected to the rank of Fellow of the AAAS, 2009; Visiting Scientist, NIMS, Tsukuba, Japan, 2010; South Carolina Section of the ACS "Outstanding Chemist 2010"; Associate Editor for Journal of Solid State Chemistry; Editor Journal of Alloys and Compounds; Elected to the rank of Fellow of the ACS, 2011; Associate Dean for Research for the College of Arts and Sciences; Southern Chemist Award, 2011; University of South Carolina Trustee Professorship Award, 2012; Vice-Chair, Solid State Chemistry Gordon Conference, 2014

Research Areas: Inorganic materials chemistry; synthesis of novel solid state materials and characterization of their physical properties; investigation of cooperative structure-property relationships; crystal growth of complex oxides and investigation of their electronic and magnetic properties.

Our research interests lie in the area of solid-state chemistry. The unifying theme in the research is the synthesis of novel solid-state materials and the correlation of structure with observed properties.

For over 20 years we have worked on the development of high-temperature solution crystal growth techniques that enable us to prepare single crystals of novel complex oxides. We have built upon our success in the adaptation and exploration of crystal growth methods and have synthesized hundreds of new compositions. A current focus is to develop the methodology to grow larger than millimeter-sized crystals for single crystal neutron diffraction experiments at the Spallation Neutron Source at Oak Ridge National Laboratory. We use crystal growth methods in the majority of our research projects.

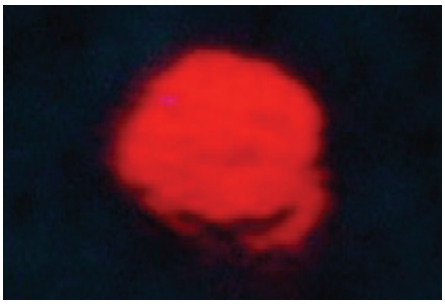

Figure 1. Optical image of the red room temperature photoluminescence in $EuKNaTaO_5$

We are developing new complex oxides in novel structure types that are highly luminescent and focus on complementary crystal growth approaches that are designed to create different classes of luminescent materials for solid-state lighting applications, including: a) the use of high temperature solutions to grow new complex rare earth containing oxides for solid state lighting and upconversion applications; b) the use of lower temperature hydrofluxes to create intrinsically luminescent oxides containing d^0 transition elements and c) the use of fluxes stable under highly reducing conditions for the crystal growth of complex Eu^{2+} containing phosphors. These three approaches will permit the directed synthesis of oxides having specific mixed rare earth contents, and allow for the fine-tuning and synthetic control of their optical properties.

We have pioneered a new research direction, the growth of complex uranium-containing oxide and fluoride crystals for fundamental and practical reasons. In general, we utilize two complementary approaches to achieve the synthesis of new complex uranium-containing oxides and fluorides based on 1) the synthesis of polycrystalline powders having compositions predicted by radius ratio rules and 2) a materials discovery approach based on crystal growth from high-temperature solutions. The synthesis of both- small, high-quality crystals containing U(VI), U(V) and U(IV) cations for structure analyses and large, high-quality crystals for use in oriented magnetic measurements and single crystal neutron diffraction experiments is on-going.

Solid oxide fuel cells (SOFCs) offer the promise of significantly increased efficiency for power delivery. In order for these systems to become a reality, improved anode materials are essential. We are investigating perovskite-based oxides, such as $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$, which exhibit high ionic and electronic conductivty, and are studying their structures and compositions under actual fuel cell operating conditions. We utilize neutron diffraction data that we collect in-situ at ORNL's Spallation Neutron Source to detect structural changes and to quantify the concentration of oxygen vacancies in these oxides. More recently we have started to explore new compositions that can cycle structurally between the perovskite and the K_2NiF_4 structure types and that can potentially be used in regenerative fuel cell systems.

Finally we collaborate on the preparation of polymer nanocomposite materials. Specifically, we are focused on the synthesis of layered oxides with high dielectric constants for the preparation of polymer composite dielectric materials for pulse power applications. We have developed approaches for preparing nanocomposite materials with extremely high weight loadings of layered nanomaterials and are testing the effect of the layered materials on the overall performance of the nanocomposite, such as dielectric constant and dielectric loss, and are extensively characterizing the physical attributes of these composite systems.

The underlying theme in all areas under investigation is the desire to understand how structure and composition affect properties, which will ultimately allow us to synthesize compounds with specific structures and, consequently, specific properties.

Representative Publications

Read, C. M.; Yeon, J.; Smith, M. D.; zur Loye, H.-C. Crystal Growth, Structural Characterization, and Optical Properties of Uranium(VI) Containing Oxychlorides, $A_2U_5O_{16}C_{12}$ (A = K, Rb), $Cs_5U_5O_{22}C_{13}$, and AUO_3Cl (A = Rb, Cs). *Cryst. Eng. Comm.* **2014** accepted, DOI: 10.1039/c4ce00281d.

Bugaris, D. E.; Hodges, J. P.; Huq, A.; Chance, W. M.; Heyden, A.; Chen, F.; zur Loye, H.-C. Investigation of the high-temperature redox chemistry of $Sr_2Fe_{1.5}Mo_{0.5}O_{6-d}$ via *in situ* neutron diffraction. *J. Mater. Chem. A* **2014**, 2, 4045-4054.

Yeon, J.; Smith, M. D.; Tapp, J.; Möller, A.; zur Loye, H.-C. Application of a Mild Hydrothermal Approach Containing an In Situ Reduction Step to the Growth of Single Crystals of the Quaternary U(IV)-containing Fluorides $Na_4MU_6F_{30}$ (M = Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, and Zn^{2+}) Crystal Growth, Structures, and Magnetic Properties. *J. Am. Chem. Soc.* **2014**, 136, 3955–3963.

Bugaris, D. E.; Smith, M. D.; zur Loye, H.-C. Hydroflux Crystal Growth of Platinum Group Metal Hydroxides: $Sr_6NaPd_2(OH)_{17}$, $Li_2Pt(OH)_6$, $Na_2Pt(OH)_6$, $Sr_2Pt(OH)_8$, and $Ba_2Pt(OH)_8$. *Inorg. Chem.* **2013**, 136, x 3836-3844.

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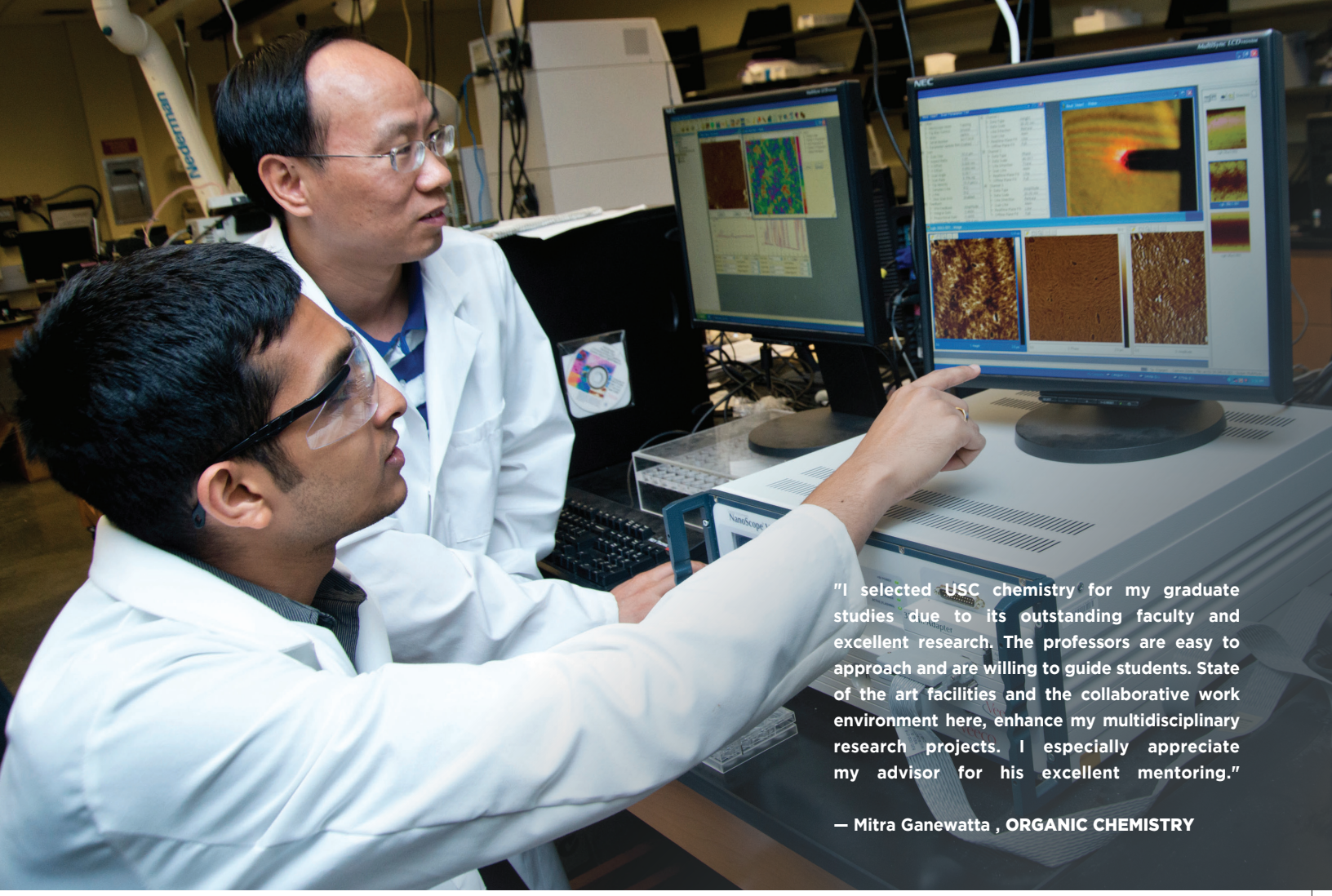
Chance, W. M.; Bugaris, D. E.; Sefat, A. S.; zur Loye, H.-C. Crystal Growth of New Hexahydroxometallates Using a Hydroflux; *Inorg. Chem.* **2013**, 52,11723-11733.

Bugaris, D. E.; zur Loye, H.-C.; Materials Discovery by Flux Crystal Growth: Quaternary and Higher Oxides", *Angew. Chem. Int. Ed.* **2012**, 51, 3780-3811.

zur Loye, H.-C.; Zhao, Q.; Bugaris, D. E.; Chance, W. M. 2H-Perovskite Related Oxides: Synthesis, Structures and Predictions. *Cryst. Eng. Comm.* **2012**, 14, 23-39.



"I selected USC chemistry for my graduate studies due to its outstanding faculty and excellent research. The professors are easy to approach and are willing to guide students. State of the art facilities and the collaborative work environment here, enhance my multidisciplinary research projects. I especially appreciate my advisor for his excellent mentoring."

— Mitra Ganewatta , ORGANIC CHEMISTRY

DEVELOPING AS A SCIENTIST

Our Ph.D. program focuses on hands-on research to prepare you to become an independent researcher in either an industrial or academic setting. During the first year, you will spend a large part of your time taking advanced course work, but thereafter, you will spend most of your time in the laboratory doing cutting-edge research. You might construct molecular wires for connecting nanoscale electronics or unravel the diabetes-related glycalation of proteins. The importance of the research done at USC is reflected in strong funding by a variety of granting agencies.

"THE DEPARTMENT TYPICALLY RECEIVES **$4 MILLION** ANNUALLY IN RESEARCH GRANTS."

In addition to developing your own research skills, you will participate in a worldwide scientific community that is advancing the frontiers of knowledge. You will publish papers on your work in major scientific journals. The department also encourages and supports your attendance at national and international conferences to present your work to other interested scientists. An active seminar program brings in top scientists from around the world to discuss their work with all members of the department.

You will learn a great deal about research from the thesis advisor that you choose from the faculty. However, you will also learn from advanced graduate students, postdocs, and visiting scientists who work with you in the same research group. These groups, typically consisting of 3–10 researchers working on closely related projects, expose you to the skills and experiences of a variety of other scientists.

Communications skills are also an important part of your development. You will give presentations to your research group and to your division of the department. Every spring, the department holds a poster competition for advanced students, with the finalist presenting a departmental seminar and going on to a University-wide competition. With this experience, you will approach presentations outside the University with confidence.

"EACH YEAR OUR GRADUATE STUDENTS MAKE DOZENS OF PRESENTATIONS"

SOCIETY FOR THE ADVANCEMENT OF THE CHEMICAL SCIENCES

The Society for the Advancement of the Chemical Sciences is an active, growing organization of graduate students in the department. The society was started in 1975 to aid members in their academic and social development and to encourage the exchange of ideas in the chemical sciences between the department's students and the scientific community.

Each year, the society's members select and sponsor a seminar speaker who has made outstanding contributions to chemistry and has influenced the chemical community. Past speakers have included such notables as Nobel Laureates Sir Geoffrey Wilkinson, Roald Hoffman, and William Lipscomb.

The society arranges for its speakers, and other speakers sponsored by the department, to be available to members in small group meetings and individual conferences. Members attend luncheon meetings each Friday with the departmental seminar speakers. This personal interaction with invited speakers is one of the most meaningful activities enjoyed by members.

Fun and recreation are also provided for society members. Each semester, members organize intramural teams and sponsor several parties, including a picnic each August to welcome incoming graduate students.

AMERICAN CHEMICAL SOCIETY POLY/PMSE

The student chapter of the American Chemical Society POLY/PMSE division is one of less than 10 student chapters nationwide. Founded in 2010 the chapter has already grown to incorporate over 30 active members of not only graduate students but undergraduates as well. The chapter was started in order to bring focus to polymer and materials science research done at USC as well as to expose students to opportunities and speakers outside of academia.

Each year, the organization funds and organizes a networking event that brings together students and professionals in academia, industry, and government labs. The students are given the opportunity to present their research at a poster session followed by a panel discussion to allow students to ask questions about careers in the panel members' respective areas. Afterwards, students and panel members are invited to dinner in order to continue discussion of research and careers in chemistry in a more relaxed setting.

While the networking event is the main feature of the year for most students, the student chapter also invites at least one guest speaker whose research in polymer science has influenced the polymer and materials science research community. Past speakers include Karen Wooley of Texas A&M, Linda Schadler of RPI, Sanat Kumar of Columbia University, and Tim Long of Virginia Tech.

Lastly, social events are planned throughout the year including cookouts, "pig pickins", bowling, and even paintball. This ensures that the most readily available network, the one within USC, isn't overlooked. All events, both professional and social, are attended by members whose research focuses on materials spanning multiple departments including chemical and biomedical engineering.

"I came to USC because of the research facilities and the faculty. I feel that the professors here are incredibly talented and can push me to develop new skills and knowledge which will aid me in the future."

—Bobby Barker, **PHYSICAL CHEMISTRY**

SEMINAR PROGRAM

Departmental seminars occur weekly and feature outstanding speakers from industry and other institutions.

Divisional seminars are offered by each of the five divisions of the department. These seminars are given by visitors from industry and academia as well as by first- and second-year graduate students delivering their required seminars.

H. Willard Davis Lectures honor a former chair of the department who retired in 1977. The 2013–2014 lecturer was Dr. Peidong Yang of the University of California at Berkeley.

Ronald R. Fisher Lectures in the Biochemical Sciences honor a former chair of the department who died in 1985. The 2013-2014 lecturer was Dr. John Johnson of the Scripps Institute.

Guy Fleming Lipscomb Lectures in Chemistry and Biochemistry honor a former department chair and founder of the Continental Chemical Company and Anchor Continental. The 2013-2014 lecturer was Dr. Miodrag Grbic of the University of Western Ontario.

Charles William Murtiashaw III Lectures honor a USC graduate who was a human disease researcher with Pfizer Inc. The spring 2013 lecturer was Dr. Robert M. Waymouth of Stanford University.

Frederick M. Weissman Lectures in Analytical Chemistry honor a 1936 graduate and distinguished neurologist. The 2013–2014 lecturer was Dr. Richard Zare of Stanford University.

STUDENT SERVICES

HOUSING

On-Campus Housing. A limited number of convenient University housing units are available for married graduate students. Married students have their choice of one-, two-, or three-bedroom unfurnished apartments at several locations ranging from $625 to $990 per month. For details, rates, and an application, contact the University Office of Graduate and Family Housing at 803-777-4571, e-mail: safmgrd@mailbox.sc.edu, or go Online to http://www.housing.sc.edu/famgrad.html

Off-Campus Housing. In general, quality rental housing is plentiful in the greater Columbia area. The average one-bedroom apartment close to campus costs approximately $600 per month, while the average two-bedroom apartment costs about $800. The Off-Campus Housing Service provides many support services, including assistance in locating housing, roommates, and rooms for rent. For additional information, visit the Web site at: https://offcampushousing.sc.edu

EMPLOYMENT OPPORTUNITIES FOR STUDENTS' SPOUSES

Many graduate student spouses find part- or full-time employment with the University. Information on University employment can be obtained by visiting the web at http://hr.sc.edu/employ.html. If you have questions, you can call the Employment Office at 803-777-3821. In addition, the South Carolina Department of Employment and Workforce operates several Columbia-area job banks that list a wide variety of employment opportunities. After you arrive in Columbia, visit the South Carolina Employment Service at 700 Taylor Street. The job bank office is open from 8 a.m. to 5 p.m. Monday through Friday. Their Web site is http://dew.sc.gov.

"**Health Insurance:** All graduate students at the University are required to have health insurance. You can either show that you have a comparable existing health plan, or obtain it at a reduced group rate through the University."

FINANCIAL SUPPORT

TEACHING ASSISTANTSHIPS

You will probably receive a teaching assistantship for your first year in the Ph.D. program. These appointments normally involve supervision of undergraduate chemistry laboratories or recitation sections and require approximately 12 hours per week (including preparation and grading). The department provides intensive teacher training and pairs new teachers with experienced peer mentors. Teaching assistantships carry a stipend of $24,000 for students entering in 2014. In addition, the department will pay teaching assistants' tuition.

RESEARCH ASSISTANTSHIPS

After your first year, you will probably be supported by a research assistantship with your research director so that you can devote full time to your research. Research assistantships carry a stipend of $24,000 for students entering in 2014. In addition, the research grant will pay research assistants' tuition. The cost of living in the metropolitan Columbia area is typically less than comparably sized cities on the East Coast, especially for housing.

FELLOWSHIPS

Each year, the University selects students to receive fellowships sponsored by federal programs, and these fellowships replace a research or teaching assistantship. Prospective graduate students with superior records will automatically be considered for these fellowships.

Prospective graduate students will also be considered automatically for departmental fellowships given in addition to a teaching or research assistantship. The Teague Fellowships honor Professor Peyton C. Teague, an organic chemist on our faculty who worked closely with the graduate program for many years. These fellowships are awarded to the most promising entering graduate students and provide supplements ranging from $1,000 to $4,000. The Murtiashaw Fellowship in Organic Chemistry honors Charles Murtiashaw III, a human disease researcher with Pfizer who received his Ph.D. degree in our department. One Murtiashaw Fellow is selected each year from applicants who indicate an interest in organic chemistry. The fellowship provides a supplement of $3,000. Other fellowships include the IRIX/David L. Coffen Fellowship, the Jerome D. Odom Fellowship in Chemistry, and USC Presidential Doctoral Fellowships.

Entering graduate students may also ask to be considered for the Summer Research Internship Program. Summer interns, called Copenhaver Scholars, serve as research assistants for up to 10 weeks and earn up to $5,800 for the summer. The program honors James Copenhaver, a former faculty member in organic chemistry who encouraged undergraduate research.

RECREATION IN AND AROUND COLUMBIA

The Columbia area provides a variety of activities for the outdoor enthusiast. Water sports, including boating, water skiing, wind surfing, sailing, fishing, and swimming, can be enjoyed year round. There are several large lakes nearby, three rivers course through the city, and the ocean is two hours away. Metropolitan Columbia has been named one of the top 10 canoe towns in the country by Paddler Magazine. Campers and hikers can drive to the Congaree National Park or Smokey Mountains. Golfers can choose from more than 20 area courses, many offering reduced student rates.

To help you take advantage of all of the outdoor opportunities, there are more than 50 active University clubs for baseball, football, canoeing, flying, sailing, skiing, scuba diving, and other sports. Students and faculty also have available, at no charge, University athletic facilities that include courts for handball, tennis, racquetball, volleyball, basketball, and squash, stations for cardiovascular and strength training, climbing walls, multipurpose sport fields, and indoor and outdoor Olympic-sized swimming pools. The Strom Thurmond Wellness and Fitness Center provides a world-class facility, which is unequivocally the best of its type in the country on a college campus. The Department of Chemistry and Biochemistry also fields intramural teams in basketball, soccer, softball, and several other sports.

As the state capital and home of the University, Columbia is a center of cultural activities in South Carolina. In addition to the University's Department of Theatre and Dance, there are several active theatre groups in the vicinity that offer exciting and varied presentations of the classics, comedy, and experimental theatre. The Koger Center for the Arts on the USC campus presents nationally and internationally recognized artists and groups. It is also the home of the USC Symphony and Chamber Orchestras, the South Carolina Philharmonic, and the Columbia City Ballet.

The Riverbanks Zoo recognized as one of the 10 best zoos in the country is an exceptional experience for all ages. It is home to more than 2,000 animals that represent more than 350 species from around the world. Each animal is seen in a living area resembling its natural habitat. Picnic areas and nature trails surround the zoo. Adjoined to the zoo the Riverbanks Botanical Garden was recognized as one of 20 great public gardens across America and features more than 4,200 species of native and exotic plants. Composed of the Asian, Bog, Dry, and Old Rose themed gardens, the gardens are constantly updated with year-round blooming species.

The Columbia Museum of Art, located near the campus, contains an important part of the Kress Collection of Renaissance, Baroque, and 18th-century art. McKissick Museum, on the University's historic Horseshoe, is a recognized center for folk art research and houses several permanent collections. The State Museum, also near the campus, houses a wide array of science, technology, and history exhibits.

COLUMBIA AND SOUTH CAROLINA INFORMATION

Welcome packets containing city and state maps, historical information, and current events calendars, as well as business, school, childcare, and recreational information, can be obtained by calling the Greater Columbia Chamber of Commerce at 803-733-1155 or by visiting www.columbiachamber.com, http://www.columbiacvb.com, and http://vistsc.com websites. The University visitor center provides a tour of the USC campus and can be contacted through http://www.sc.edu/visit/ website.

S.C. travel guides, including attractions, maps, and information about specific regions in the state, can be obtained by visiting http://www.columbiacvb.com or website of S.C. Department of Parks, Recreation, and Tourism at http://www.scprt.com. A visitor guide can be requested through http://www.columbiacvb.com.

FOR FURTHER INFORMATION CONTACT:

Graduate Admissions Committee

Department of Chemistry and Biochemistry
631 Sumter St.
University of South Carolina
Columbia, SC 29208

Telephone: 803-777-2579

Toll-free: 800-868-7588

Fax: 803-777-9521

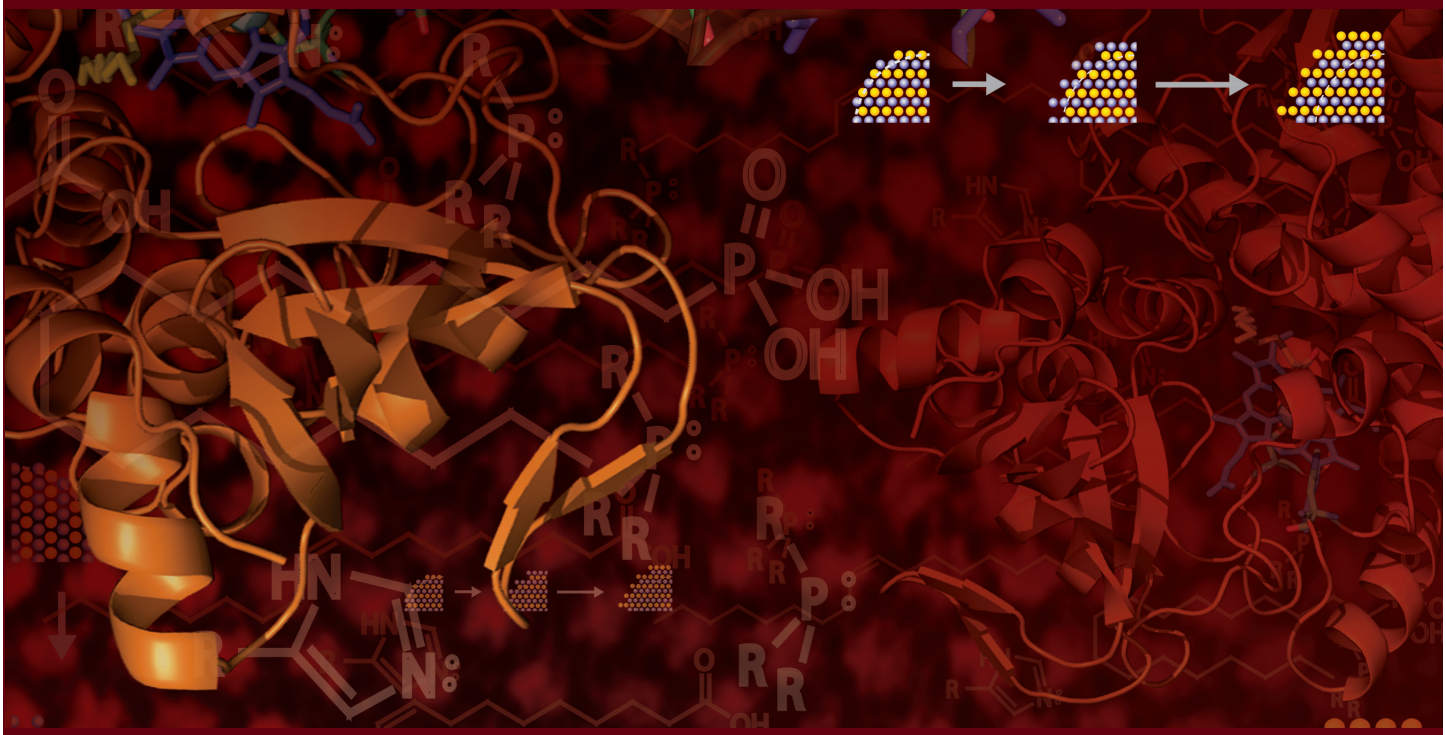
E-mail: chemgrad@mailbox.sc.edu

WWW.CHEM.SC.EDU

Please consult our Web site for additional information, including updates on faculty and staff appointments, honors, and awards; information about current graduate students, research professors, postdoctoral associates, and emeriti faculty; and complete lists of past seminar speakers.

10297 University Publications 10/10
revised by Jemimah Ekeh, Chemistry 6/14

www.chem.sc.edu



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