Chemistry Seminars
Spring, 2010

Tuesdays at 11:00-12:00
Thursday, October 15 at 11:00-12:00

Classroom Building 170
Seminar Program

February 2
Phil Crews
Department of Chemistry, University of California, Santa Cruz
Marine Natural Products at UCSC — Milestone Discoveries & Lessons Learned

February 9
William T. Stringfellow
Geochemistry Department, Lawrence Berkeley National Laboratory
Water quality, Cyanobacteria, and Cyanobacteria toxins

February 16
Mark J. Kurth
Department of Chemistry, University of California, Davis
TBA

February 23
John I. Brauman
Department of Chemistry, Stanford University
Hydrogen Bonding: Acidity, Basicity, and Effects on Reactivity

March 2
Patricia C. Babbitt
Department of Biopharmaceutical Sciences, University of California, San Francisco
A Global View of Enzyme Superfamilies: Promiscuity & the Evolution of New Functions

March 16
Ken Moody
Chemical Sciences Division, Lawrence Livermore National Laboratory
Forensic Radiochemistry

March 23
Patricia LiWang
School of Natural Sciences, University of California, Merced
Structural and Functional Studies of HIV Inhibitors
March 30
Michael D. Fayer  
*Department of Chemistry, Stanford University*  
Watching Ultrafast Molecular Motions in Liquids, Molecules, and Proteins

April 6
T. Don Tilley  
*Department of Chemistry, University of California, Berkeley*  
Catalysts for the Production of Chemical Fuels via Solar Energy Conversion

April 13
Craig Vierra  
*Department of Biological Sciences, University of the Pacific*  
Unraveling Spiderman's Glue Silk

April 20
Robert W. Carling  
*Transportation Energy Center, Sandia National Lab*  
Sandia’s Combustion Research Facility

April 27
Joel H. Parks  
*Rowland Institute at Harvard, Harvard University*  
Fluorescence Lifetime Probe of Biomolecular Conformations

May 4
Peter B. Armentrout  
*Department of Chemistry, University of Utah*  
Solvation, Nanochemistry, and Biochemistry in the Gas Phase
Bio: Phillip Crews is currently a faculty member at the University of California Santa Cruz (UCSC) and holds the rank of Disguised Professor of Chemistry. His research labs are in the Department of Chemistry and Biochemistry and other affiliations include those with the UCSC Institute of Marine Sciences and the California Institute for Quantitative Biomedical Research, called QB3. Phil Crews received a B.S. in Chemistry at UC Los Angeles, a Ph.D. in Chemistry at UC Santa Barbara and was an NSF posdoctoral fellow at Princeton University. His entire academic career has been spent at UCSC, a remarkable campus that was established in 1965.

His rigorous attention to research, education, and service for the past 38 years at U.C. Santa Cruz has positively impacted the careers of many individuals and was the basis for a promotion several years ago to status as an above scale U.C. Professor. He has published over 175 research papers in peer-reviewed journals. He is the author of the widely used textbook “Organic Structure Analysis”. He has mentored 25 Ph. D students and 9 MS students. He has sponsored 34 postdoctoral associates including visiting professors. Professor Crews is a member of the American Society of Pharmacognosy, the American Chemical Society, the American Association for the Advancement of Science, the National Organization of Black Chemists & Chemical Engineers, and the American Society of Ecology and Viticulture. Professor Crews plays a very active role in the natural products community at large. He served on the organizing committee for the 1996 ASP Annual Meeting held in Santa Cruz. He was a co-organizer of the 1998 IVth U.S. Japan Seminars in Marine Natural Products Research, and recently served as Chair of the 2008 Marine Natural Products Gordon Research Conference.

The long-term focus of the Crews group is to expand fundamental knowledge about the novel structures and the bioactivity of marine natural products. Tropical sponges are the primary marine taxa being studied in a highly collaborative program with other academic and corporate scientists. The strategy of bioassay guided isolation enables the discovery of novel compounds that are active against a variety of human diseases. Sponges gathered during expeditions to coral reefs throughout the world are the beginning point for all investigations. The role of sponge associates in the contributing to the overall chemodiversity observed illustrates the interface of this research with biology. An additional subject of interest involves the study of metabolites isolated from marine fungi grown in salt-water culture. Obtaining chemically prolific sponge-derived fungi from both shallow water and deep water organisms represents a comprehensive approach. Another dimension of this research seeks fundamental understanding of the biosynthetic pathways responsible for biologically active sponge derived polyketides, peptides and mixtures of these classes.
Marine Natural Products at UCSC — Milestone Discoveries & Lessons Learned

Phil Crews

*February 2, 11:00 AM, Classroom Building 170*

The marine natural products program begun at UC Santa Cruz (UCSC) in the early 1970’s has a rich history and continued promise for future significant discoveries. To date, almost 900 molecular structures have been established by the UCSC group from the study of marine invertebrates, especially sponges and marine-derived fungi, and these continue to captivate the interests of research groups throughout the world. Using case examples I will amplify on: (1) new scaffolds being explored for anti-cancer therapeutic lead development, (2) the continuing challenges to obtain sponge-derived compounds seemingly biosynthesized by microbial associates, (3) the potential and challenges associated with mining complex mixtures obtained from culture of marine-derived fungi.
William T. Stringfellow
Geochemistry Department
Lawrence Berkeley National Laboratory
Berkeley, CA 94720
wstringfellow@lbl.gov

Education: Ph. D., Environmental Sciences and Engineering, UNC Chapel Hill, 1994; M. S., Microbiology (minor: Aquatic Ecology), Virginia Polytechnic Institute and State University, 1984; B. S., Environmental Health, University of Georgia, 1980.


Selected Publications

Cyanobacteria blooms have impaired beneficial uses of surface waters around the world. Blooms of these microorganisms, also known as blue-green algae, can form thick mats on the surface of rivers and lakes. These mats are unsightly and typically malodorous. Blooms of these algae can contaminate drinking water, imparting a noxious taste and odor that can not be removed by conventional treatment processes. In addition to aesthetic problems, many cyanobacteria species produce toxins (cyanotoxins). Microcystin, a hepatotoxin, is one of the cyanotoxins commonly associated with blue-green algae blooms around the world. Microcystin can be harmful and at times lethal to humans, cattle, pets and aquatic wildlife. The World Health Organization has set a limit of 1μg/L microcystin for drinking water. Although blue-green algae blooms have been investigated intensively, the environmental conditions that lead to toxin production in blooms are not well understood.

In the summer of 2009, the presence of cyanobacteria in the Sacramento-San Joaquin Delta was investigated. Grab samples were collected in urban sloughs and open channels. Microscopy was used to determine biomass and type of cyanobacteria present. In situ fluorescence measurements were taken of phycocyanin, a photosynthetic pigment specific to blue-green algae, to determine if a rapid method could be developed for the monitoring of algal blooms in estuary environments. Microcystin concentration was measured using an immune assay (ELISA). Environmental conditions and water quality parameters were recorded at the time of sample collection, and grab samples were analyzed for various nutrients. Cyanobacteria were found to be present in all samples collected. A correlation was found between microcystin concentrations and blue-green algal biomass with 73% of the correlation explained by the presence of the algal genus *Microcystis*. Environmental conditions positively correlated to toxin concentration and cyanobacterial biomass included: low dissolved nitrate, low conductivity, low dissolved N to dissolved P molar ratios, low turbidity, and high dissolved silica. A clear spatial distribution pattern was found and could be related to the differing water quality of the Sacramento and San Joaquin Rivers. In situ phycocyanin measurements were not correlated to cyanobacterial biomass, in part due to the inability of sensors to detect cyanobacteria in mats and surface scums. The highest concentration of cyanobacteria and toxin was found near a major drinking water intake. The widespread distribution of cyanobacteria and cyanotoxins in the Delta suggest the possibility that large scale blooms could occur in the future, but current microcystin concentrations are below the 1μg/L limit set by the World Health Organization.
Mark J. Kurth

Department of Chemistry
University of California, Davis
Davis, CA 95616

kurth@chem.ucdavis.edu

Education:
XXX

Mark J. Kurth

February 16, 11:00 AM, Classroom Building 170

The
John I. Brauman  
Department of Chemistry  
Stanford University  
Stanford, CA 94305  
brauman@stanford.edu

Bio: John Brauman was born in Pittsburgh, PA in 1937. He attended M.I.T. (S.B., 1959) and the University of California at Berkeley (Ph.D., 1963). He was a National Science Foundation Postdoctoral Fellow at UCLA, then took a position at Stanford University where he is J. G. Jackson - C. J. Wood Professor of Chemistry, Emeritus. He was Department Chair, Associate Dean for Natural Sciences, and has been Associate Dean of Research since 2005. He also currently serves as the Home Secretary of the National Academy of Sciences. 
Brauman has received a number of awards including the American Chemical Society Award in Pure Chemistry, Harrison Howe Award, Guggenheim Fellowship, R. C. Fuson Award, Arthur C. Cope Scholar Award, the James Flack Norris Award in Physical-Organic Chemistry, the National Academy of Sciences Award in Chemical Sciences, the Linus Pauling Medal, the Willard Gibbs Medal, and the National Medal of Science. He is a member of the National Academy of Sciences, the American Academy of Arts and Sciences, the American Philosophical Society, a Fellow of the American Association for the Advancement of Science, and an Honorary Fellow of the California Academy of Sciences. He received the Dean's Award for Distinguished Teaching from Stanford University. Brauman has served on many national committees and advisory boards. He was Deputy Editor for Physical Sciences for SCIENCE from 1985 to 2000 and is currently the Chair of the Senior Editorial Board. 
Brauman's research has centered on structure and reactivity. He has studied ionic reactions in the gas phase, including acid-base chemistry, the mechanisms of proton transfers, nucleophilic displacement, and addition-elimination reactions. His work includes inferences about the shape of the potential surfaces and the dynamics of reactions on these surfaces. He has made contributions to the field of electron photodetachment spectroscopy of negative ions, measurements of electron affinities, the study of dipole-supported electronic states, and multiple photon infrared activation of ions. He has also studied mechanisms of solution and gas phase organic reactions as well as organometallic reactions and the behavior of biomimetic organometallic species.
Hydrogen Bonding: Acidity, Basicity, and Effects on Reactivity

John I. Brauman

February 23, 11:00 AM, Classroom Building 170

Hydrogen bonds play a critical role in molecular recognition and binding. Many biological and chemical systems depend on hydrogen bonding to effect specificity and enhance catalytic efficiency. Our understanding of hydrogen bonding, in general, has been limited by the variety of chemical systems that have been studied.

We have studied a variety of hydrogen bonded negative ion complexes in the gas phase, using ion cyclotron resonance spectroscopy. We explore the validity of some common assumptions. Does the structure of the complex depend on the relative acidity of the constituent components? Does the correlation of H-bond strength vs. acidity reflect the structure of the complex or the degree of proton transfer in the complex? We also examine some hydrogen bonded complexes in terms of their thermodynamic stability and kinetic reactivity.
Patricia C. Babbitt

Department of Biopharmaceutical Sciences, UC San Francisco
San Francisco, CA 94143

babitt@cgl.ucsf.edu

Education: 08
A Global View of Enzyme Superfamilies: Promiscuity & the Evolution of New Functions

Patricia C. Babbitt

March 2, 11:00 AM, Classroom Building 170

The
Bio: Ken Moody received a Bachelor of Science degree in Physical Chemistry from the University of California, Santa Barbara, in 1977. He attended graduate school in Berkeley, where he studied under Nobel Laureate Glenn Seaborg (the discoverer of plutonium), and received a Ph.D. in 1983, specializing in actinide radiochemistry. He spent two years at the Gesellschaft für Schwerionenforschung in Germany, performing heavy element experiments. He has worked at the Lawrence Livermore National Laboratory since 1985, making radiochemical diagnostic measurements in support of various national security programs. Currently, in addition to his programmatic assignments, he is the senior member of the Livermore Heavy Element group, performing basic research on the elements at the extreme limits of the periodic table, in collaboration with physicists at accelerator laboratories in the former Soviet Union. He is codiscoverer of four dozen heavy isotopes and six chemical elements, and is a coauthor of a recent book on nuclear forensic analysis.
Radiochemical signatures inherent in samples of plutonium or uranium give clues about the origin of the material. Such information can be quite important when trying to determine the source of smuggled nuclear materials interdicted by law enforcement personnel. The fact that significant amounts of illicit weapons-grade materials have been seized in Europe attests to the importance of this problem. Ingrowth of daughter nuclei in radioactive decay provides a means by which the age of a sample can be determined. Excess of a given radionuclide over the amount produced by decay provides a clue as to the chemical processes used in manufacturing the sample, while the abundances of the isotopes in the matrix give information on the previous relationship between the production facility and the nuclear fuel cycle. Results from several real-world samples will be used to illustrate these points.
Bio: Patricia LiWang received her undergraduate degree from the Massachusetts Institute of Technology and her Ph.D. from Harvard University. After a post doctoral fellowship at the National Institutes of Health, she went onto the faculty at Purdue University and then at Texas A&M University. She has recently moved her laboratory to the University of California at Merced, where the group has pursued the study of chemokines as well as a broad variety of HIV inhibitors.

Selected Publications:


About 2.7 million people are infected with HIV each year, and there are about 33 million people living with AIDS. There is a great need both for new therapies to treat infected people as well as therapies that may prevent infection. HIV entry inhibitors may fulfill both roles and are particularly promising as microbicides that can be used to inhibit infection by sexual contact. This would be particularly helpful to prevent the spread of HIV, especially in developing countries. The design of entry inhibitors is one of the most exciting challenges in HIV inhibition, and the LiWang group is working toward highly potent HIV entry inhibitors with several types of proteins. We study both the structure and function of proteins, using techniques ranging from NMR to in vitro HIV cell fusion assays. This presentation will discuss some of our recent work to study HIV entry inhibitors as well as our work with related proteins that are involved in inflammation.
Bio: Professor Michael D. Fayer is the D. M. Ehram and E. C. Franklin Professor of Chemistry at Stanford University. For many years, Professor Fayer has been a pioneer in the development and application of ultrafast non-linear laser techniques. In large part due to his work, ultrafast nonlinear and coherent spectroscopic techniques such as transient gratings, photon echoes, and vibrational echoes have become powerful techniques for studying fast molecular processes, intermolecular interactions, and structure in complex molecular systems. His work has had a profound impact on modern physical chemistry, biophysics, and materials science, and his methods and approaches to the examination of problems involving dynamics and interactions in molecular systems have spread worldwide. Michael Fayer is a member of the National Academy of Sciences of the United States of America and of the American Academy of Arts and Sciences. He has won a number of national and international awards including the Ellis R. Lippincott Award given by the Optical Society of America, the E. Bright Wilson Award for Spectroscopy given by the American Chemical Society and the Earl K. Plyler Prize for Molecular Spectroscopy given by the American Physical Society.
Watching Ultrafast Molecular Motions in Liquids, Molecules, and Proteins

Michael D. Fayer

March 30, 11:00 AM, Classroom Building 170

The natural systems we encounter in daily life, from water to the most complex biological structures, are composed of molecular subunits that are inherently small, that is, the nanometer length scale. Because molecules are small, the time scale for molecular motions is very fast, on the order of picoseconds. Constantly evolving inter and intramolecular structures make molecular processes possible. To understand the complex molecular systems that pervade our environment, we need methods that can examine the fast evolution of molecular systems without changing the properties of the systems. Recent technological and theoretical developments have produced a new experimental tool, Ultrafast Two Dimensional Infrared (2D IR) Vibrational Echo Chemical Exchange Spectroscopy, which has achieved this goal. The method makes it possible to study fast molecular motions under thermal equilibrium conditions. The 2D IR chemical exchange experimental methodology is described, and how information is extracted from the 2D IR data is explained. Novel results on liquid, molecular, and protein dynamics are presented.
T. Don Tilley
Department of Chemistry
University of California, Berkeley
Berkeley, CA 94720
tdtilley@berkeley.edu

Education
Ph.D. Chemistry (1982): University of California, Berkeley
B.S. Chemistry (1977): University of Texas, Austin

Academic Career
1981-1983: Postdoctoral research with Profs Grubbs and Bercaw (Caltech) and Profs Pino and Venanzi (ETH, Zürich) in a US-Swiss program
1983-1988: Assistant Professor, Department of Chemistry, UC San Diego
1988-1990: Associate Professor, Department of Chemistry, UC San Diego
1990-1994: Professor, Department of Chemistry, UC San Diego
1994- : Professor, Department of Chemistry, UC Berkeley
1994- : Senior Faculty Scientist, Lawrence Berkeley National Laboratory

Honors and Awards

Service
Chair of the ACS Division of Inorganic Chemistry (2003)
North American Associate Editor (Inorganic, Organometallic and Materials Chemistry), Chemical Communications (2005-present).

Publications
340 in books or scientific journals; 4 in press; 3 patents
The integration of photovoltaics and catalysts into a useful system for solar energy conversion will require a number of advances, including the development of high-efficiency, nanoscaled photovoltaic units, the discovery of inexpensive electrocatalysts for the half-reactions of interest, and the incorporation of efficient catalysts onto the surfaces of the photovoltaics. For schemes based on water oxidation, it is possible to envision catalysts derived from molecular transition metal complexes, or from inorganic solid-state materials. The best molecular systems reported to date utilize ruthenium centers, and more useful catalysts based on first-row metals seem possible given the known behavior of the tetranuclear μ-oxo-bridged manganese center as the oxygen-evolving complex (OEC) in photosystem II (PSII). Transition metal oxides represent potential inorganic electrocatalysts for water oxidation. As part of a program to identify structural and compositional factors that lead to efficient water oxidation, the size- and shape-dependence of metal oxide nanostructures on electrocatalytic oxygen evolution has been targeted. Recent interest has also focused on the synthesis of proton reduction catalysts as additional components in a solar-to-fuel system. Along these lines, the synthesis and structure of diiron proton reduction electrocatalysts, inspired by the iron-only hydrogenases, have been targeted. They contain, unlike the vast majority of hydrogenase mimics, structurally rigid dithiolates that are built upon naphthalene-1,8-dithiolates.
Education:
Unraveling Spiderman's Glue Silk

Craig Vierra

April 13, 11:00 AM, Classroom Building 170

Despite
Dr. Bob Carling is the director of the Transportation Energy Center at Sandia National Laboratories in California. In this role, he oversees the Combustion Research Facility (CRF), the Department of Energy’s (DOE’s) premier collaborative research center for combustion science and technology. Dr. Carling is also responsible for guiding Sandia’s transportation energy research and development (R&D) beyond combustion to other promising ventures, such as hydrogen, advanced batteries, and alternative fuels.

Dr. Carling joined Sandia in 1976 as a member of the technical staff. During his early years at Sandia, he conducted research on molten nitrate salts and other chemical systems for solar energy transfer and storage. Dr. Carling’s management career began in 1983 when he was promoted to become the supervisor of the Exploratory Chemistry Department.

In 1986, Dr. Carling moved to the CRF. He assumed management responsibility for a DOE/Department of Defense program on energetic materials. He then managed the Engine Combustion Department and was a key participant in the Partnership for a New Generation of Vehicles, an initiative between DOE and the U.S. Council for Automotive Research (a consortium of GM, Ford, and Chrysler) to improve combustion efficiency and reduce pollutants. Dr. Carling then became a CRF senior manager, overseeing the CRF’s Visitor Program and R&D projects in microfluidics, remote sensing, and the chemical sciences.

In 2005, Dr. Carling was promoted to become the director of the Physical and Engineering Sciences Center. The center specialized in materials and engineering sciences R&D, particularly in the areas of surety solutions, hydrogen science and technology, and science-based advanced-concepts engineering. The center’s projects, which ranged from fundamental research to applied engineering, were especially pertinent to the work conducted by Sandia’s Energy and Nuclear Weapons strategic management units. Dr. Carling assumed his current role as director of the Transportation Energy Center in 2008.

Dr. Carling holds a bachelor’s degree in biology from Olivet College, a master’s degree in chemistry from Oakland University, and a PhD in physical chemistry from the University of Michigan. He is a member of the board of directors for the Bay Area Science and Innovation Consortium.
Sandia’s Combustion Research Facility

Robert W. Carling

April 20, 11:00 AM, Classroom Building 170

Sandia’s Combustion Research Facility (CRF) has been the international research and development leader in combustion for more than 25 years. In this presentation I will discuss a bit of the history of the CRF and our impact in the energy and fuels arena. Given the challenges the country and the world face in energy and climate, I will discuss our plans for the future, specifically related to advanced internal combustion engine efficiency and emissions. You will learn that chemistry will play a key role in whatever success we have.
Joel H. Parks

Rowland Institute at Harvard
Harvard University
Cambridge, MA 02142

parks@rowland.harvard.edu

Education: Ph.D. Physics, Massachusetts Institute of Technology, Cambridge (1959); B.S. Physics, Massachusetts Institute of Technology, Cambridge (1969).


Representative Publications:

Fluorescence Lifetime Probe of Biomolecular Conformations

Joel H. Parks

April 27, 11:00 AM, Classroom Building 170

Methods have been developed to measure the fluorescence lifetime vs temperature of trapped, gas phase biomolecular ions derivatized with a fluorescent dye. A quenching interaction between the dye excited state and a tryptophan residue is sensitive to thermally driven spatial fluctuations of the residue. Measurements and molecular dynamics calculations for different sequences of polyproline peptides indicate that the quenching rate vs temperature curves strongly depend on the sequence as a result of these spatial fluctuations. The talk will introduce these fluorescence methods and present their application to the study of conformational dynamics of larger biomolecules. Vancomycin-peptide noncovalent complexes in the 1+ charge state were studied as a function of temperature for different peptide chiralities. Fluorescence quenching rates of the complex were found to be stereoselective for different peptide chiralities. A variation in quenching resulting from a change in the chirality of a single amino acid was readily detectable. Molecular dynamics analyses were performed for complexes formed by different stereoisomers. These calculations indicate increased flexibility of the noncovalent complex structure which is correlated with the observed reduction of quenching rates. Fluorescence measurements were also performed for the Trp-cage protein to compare quenching rates in different charge states. Measurements of sequences including single-point mutations infer the presence of a salt-bridge structure in the 1+ charge state and its absence in both 2+ and 3+ states. Molecular dynamics structures of Trp-cage indicate that a salt bridge in the 1+ charge state produces more compact conformations leading to the larger quenching rates found experimentally. In each of these experimental studies the fluorescence quenching rates were found to be consistent with changes in structure, induced either by intermolecular or intramolecular interactions.
Peter B. Armentrout

Department of Chemistry
University of Utah
Salt Lake City, UT 84112

armentrout@chem.utah.edu

Bio: B.S., Chemistry, Case Western Reserve University (1975); Ph.D., Chemistry, California Institute of Technology (1980); Postdoctoral Member of Technical Staff, Bell Laboratories (1980-1981); Assistant Professor of Chemistry, University of California, Berkeley (1981-1987); Associate Professor of Chemistry, University of Utah (1987-1989); Professor of Chemistry, University of Utah (1989-1998); Distinguished Professor of Chemistry, University of Utah, (1998-present); Cannon Fellow (2003-present); Chair, Department of Chemistry, University of Utah (2001-2007); Visiting Scientist, Fakultät für Physik der Universität Freiburg, Germany (1992); Professeur d’Invitee, Universitaire de Paris-Sud, France (1994); Japan Society for the Promotion of Science (JSPS) Fellow (1999); Professeur d’Invitee, Universite de Pierre et Marie Curie (2008). Camille and Henry Dreyfus Grant for Newly Appointed Faculty in Chemistry (1981); Presidential Young Investigator Award, National Science Foundation (1984-1989); Alfred P. Sloan Research Fellow (1986-1990); Camille and Henry Dreyfus Teacher-Scholar (1987-1992); Outstanding Undergraduate Teaching Award, Chemistry Department, University of Utah (1988-1989); Fellow of the American Association for the Advancement of Science (1992); Buck-Whitney Award, American Chemical Society Eastern New York Section (1993); Distinguished Research Award, University of Utah (1994); Fellow of the American Chemical Society (1997); Outstanding Alumnus of the Year, Department of Chemistry, Case Western Reserve University (2004); Freiser Memorial Lecture, Purdue University (2007); Field and Franklin Award for Outstanding Achievement in Mass Spectrometry, American Chemical Society (2009).

Representative Publications

- “Guided ion beam and theoretical studies of the reaction of Ag$^+$ with CS$_2$: Gas-phase thermochemistry of AgS$^+$ and AgCS$^+$ and insight into spin-forbidden reactions” Armentrout, P. B.; Kretzschmar, I. *J. Chem. Phys.* 2010, 132, 024306-1-10.
The thermochemistry and dynamics of a wide range of chemical phenomena are examined using guided ion beam tandem mass spectrometry. By measuring how ion-molecule reactions depend on translational energy over a broad range, the mechanisms and energetics of these reactions can be elucidated. Examples will be given in three related areas.

1) The hydration energies of multiply charged ions are either unknown (e.g., Fe$^{2+}$, Zn$^{2+}$, and Cd$^{2+}$) or measured only for the second solvent shell (alkaline earths). Using these techniques, the thermochemistry for the inner solvent shell is measured for the first time for all these metal cations. In addition, the charge separation into hydroxides and protonated water clusters is quantitatively elucidated for the first time.

2) Reactions of cationic clusters of transition metals and their oxides provide thermodynamic information that cannot be measured in any other way. It is shown that this information can be directly related to phenomena occurring on surfaces, providing thermochemistry for catalytic reactions of broad importance.

3) The decomposition reactions of metallated and protonated amino acids are examined. This provides a “thermodynamic vocabulary” of pairwise intrinsic binding energies of metal cations to these species, elucidating how the side-chain substituents influence the interactions. In some cases, the thresholds for decomposition reactions provide insight into the mechanisms for the dissociation process, which can be related to analogous reactions of biological importance.