



ACS 239<sup>th</sup> NATIONAL MEETING DIVISION OF  
GEOCHEMISTRY



San Francisco, CA  
March 21-25, 2010

Call for Papers

The Geochemistry Division has organized the following topical oral symposia, consisting of both invited and contributed papers, and also topical and general poster sessions. **The abstract deadline is October 19, 2009. To submit your 150 word abstract, go to: [www.acs.org/meetings](http://www.acs.org/meetings)**

**Predicting Molecular Properties of the Mineral-Water Interface: Challenges and Opportunities for High Performance Computing.** Co-sponsored by the Division of Computers in Chemistry. For more information contact: *Andrey G. Kalinichev*, Michigan State University, 517-355-9715 ext. 336, [kalinich@chemistry.msu.edu](mailto:kalinich@chemistry.msu.edu). *James D. Kubicki*, Pennsylvania State University, 814-865-3951, [kubicki@geosc.psu.edu](mailto:kubicki@geosc.psu.edu). *David A. Dixon*, University of Alabama 205-348-8441, [dadixon@as.ua.edu](mailto:dadixon@as.ua.edu)

Most geochemical reactions involve fluid phases and take place at fluid-mineral interfaces or in confined spaces of mineral interlayers and nanopores. These reactions affect many important natural processes, including mineral weathering, adsorption or release of environmental contaminants in soil, drinking water quality, the fate of CO<sub>2</sub> in geologic carbon sequestration. A molecular-level understanding of the chemistry and physics of interfacial and confined aqueous solutions interacting with mineral surfaces is essential to understanding many of the crucial problems in energy and the environment. Atomistic computer simulations offer powerful tools to obtain such quantitative information. Current and emerging petascale supercomputing capabilities can provide understanding of the mineral-water interface at such level of detail that standard computational approaches (using PCs, workstations, multiprocessor clusters, etc.) are unable to achieve. This symposium will focus on the scientific challenges of large-scale geochemical computational molecular modeling and on the computational approaches to meeting those challenges.

**Aquatic Redox Chemistry: in Honor of Donald L. Macalady.** Co-Sponsored with Environmental Chemistry Division For more information: *Paul G. Tratnyek*, [tratnyek@ebs.ogi.edu](mailto:tratnyek@ebs.ogi.edu), *Timothy J. Grundl*, [grundl@uwm.edu](mailto:grundl@uwm.edu) or *Stefan Haderlein*, [haderlein@unituebingen.de](mailto:haderlein@unituebingen.de)

This symposium will highlight recent developments in the general area of aquatic redox chemistry. Major areas of interest will include interactions between iron, natural organic matter (NOM), and contaminants. Specific topics of interest include—but are not limited to—speciation and redox reactions of iron, structure and reactivity of NOM as a redox shuttle, and redox reactions that contribute to the fate of organics (e.g., pesticides and nitroaromatic model compounds) and metals (e.g., arsenic).

The symposium is timed to celebrate the diversity of contributions that Prof. Macalady has made to many of these topics. Both invited and contributed papers are planned. Invited speakers include: Janet Hering, Diane McKnight, Ken Nealson, René Schwarzenbach, Garrison Sposito, and Eric Weber.

**The Influence of Natural Organic Matter on the Fate and Transport of Metals, Colloids and Nanoparticles in the Aquatic Systems:** Co-Sponsored with Environmental Chemistry Division  
For more information contact: *George Aiken*: [graiken@usgs.gov](mailto:graiken@usgs.gov), *Helen Hsu-Kim*, [hsukim@duke.edu](mailto:hsukim@duke.edu) or *Joseph Ryan*, [joseph.ryan@colorado.edu](mailto:joseph.ryan@colorado.edu)

Improved understanding of the geochemistry, fate and transport of metals, colloids and engineered nanoparticles is critical for assessing the ecological and human health impacts associated with these materials. Macromolecular organic matter such as humic substances and small molecular weight organics are ubiquitous in water, soil and

sediment environments. Thus, natural organic matter frequently controls metal speciation and surface charge of particles, influences sorption interactions with mineral surfaces and drives important reactions (e.g. redox and photochemical reactions) influencing the behavior of metals, colloids, and nanoparticles in aquatic systems. In this session we will focus on studies addressing the nature of chemical interactions between natural organic matter and metals (mercury, in particular), colloids and nanoparticles (both engineered and natural) and the influences these reactions have on the transport, bioreactivity, and geochemistry of these materials in the environment.

**Advancing the Science of Natural Zeolites: A Symposium in Honor of Robert S. Bowman** For more information contact: *Enid J. Sullivan*, Los Alamos National Laboratory 505-667-2889, [ejs@lanl.gov](mailto:ejs@lanl.gov).

This symposium is dedicated to Robert S. Bowman who lost his battle with cancer in June, 2009. Professor Bowman was internationally recognized for his applications of zeolite to contaminant removal for both small-scale operations in rural developing country communities, to large-scale operations for industry and large municipal water systems. This symposium will examine the potential applications of zeolite and includes topics focused on molecular scale understanding of zeolite properties to field scale applications of zeolite based processes. In addition, Professor Bowman was well known for his contributions to understanding the impact of hydrology on geochemical cycling. Papers in this area are also welcome.

**Environmental and Geochemical Aspects of Carbon Sequestration:** Co-sponsored with Environmental Chemistry Division. For More Information Contact: Daniel E. Giammar, Washington University in St. Louis, 314-935-6849, [giammar@wustl.edu](mailto:giammar@wustl.edu). Young-Shin Jun, Energy, 314-935-4539, [ysjun@seas.wustl.edu](mailto:ysjun@seas.wustl.edu). Charles J. Werth, University of Illinois at Urbana-Champaign, 217-333-3822, [werth@illinois.edu](mailto:werth@illinois.edu)

Geological carbon sequestration has the potential to mitigate anthropogenic carbon dioxide emissions that have perturbed the global carbon cycle and are impacting the global climate. Geological carbon sequestration will involve the development and deployment of technologies that couple chemical reactions and transport on very large scales. Current research is generating new information on geochemical and environmental reactions that are essential to designing sequestration strategies, predicting their performance, and assessing potential risks. Relevant processes include dissolution-precipitation reactions and other interfacial reactions at the high pressures and temperatures of sequestration formations. Multi-phase reactive transport experiments and simulations are important in predicting sequestration performance. Environmental aspects of geological carbon sequestration include monitoring and remediating leaks from formations and assessing the integrity of capping formations and well seals.

This symposium welcomes papers for presentations that describe advances in our understanding of environmental and geochemical aspects of carbon sequestration. Topics of interest include, but are not limited to, laboratory investigations of sequestration processes, field-scale characterization and assessment of sequestration systems, and modeling of reactions and transport at multiple scales.

Confirmed Invited Speakers Include: *Sally Benson* (Stanford University), *David Cole* (Oak Ridge National Laboratory), *Don DePaolo* (Lawrence Berkeley National Laboratory / University of California-Berkeley) and *Catherine Peters* (Princeton University)

**Biogeochemistry of Endocrine Disrupting Chemicals and other Emerging Contaminants in Natural Systems**  
For more information contact: Howard M. Liljestrand, University of Texas at Austin, 512-471-4604, [liljestrand@mail.utexas.edu](mailto:liljestrand@mail.utexas.edu)

The occurrence of endocrine disrupting chemicals (EDCs), personal care products, pharmaceutically active compounds and other emerging contaminants in natural and treated water is widespread. Concern regarding the impact of these contaminants on human health and the environment necessitates a greater understanding of the fate, transport and reactivity of these compounds. Recent research has shown that many of the traditional approaches that we have used to estimate reactivity, develop remediation strategies, and predict contaminant migration are not reliable for these compounds. The focus of this symposium is on developing a better understanding of the biogeochemistry of these compounds and on the development of techniques for estimating their behavior in the environment.

**Frontiers in Analytical Chemistry as Applied to Natural Organic Matter** For more information contact Rose Cory, University of North Carolina, 612-626-7981, [rmcory@email.unc.edu](mailto:rmcory@email.unc.edu)

One of the greatest opportunities for the field of analytical chemistry to advance understanding of the global carbon cycle may occur through chemical characterization of natural organic matter (NOM). NOM, one of the most complex organic mixtures on Earth, is also arguably the most important intermediate in the global carbon cycle. Interdependent biotic and abiotic transformations of NOM result in greenhouse gases and a reservoir of “leftovers”- e.g. recalcitrant material. Contributing to the difficulty in partitioning the fate of NOM in the global carbon cycle is the fact that we are unable to recognize the molecular signature of the NOM that may be oxidized to CO<sub>2</sub>, for example, or the molecular signature of the recalcitrant pool amongst the complex mixture of thousands of compounds contributing to NOM. However, advances in analytical capabilities along with multi-way data analysis techniques to deal with complex spectra, for instance, are yielding molecular information of NOM in increasing detail.

A goal of this session is to promote discussion on emerging trends in the molecular signatures of reactive and recalcitrant NOM in the context of the global carbon cycle, as obtained from the frontiers in analytical approaches including, but not limited to, high resolution mass spectrometry, nuclear magnetic resonance (NMR), X-ray absorption spectroscopy, or multi-way analysis of NOM fluorescence spectra. We also invite studies focused on new approaches to NOM characterization that emphasize molecular interactions over molecular components.

**Water and Renewable Energy Production** For more information contact: Kerry Kinney, The University of Texas at Austin, Austin, TX 78712, Phone: 512-232-1740, [kakinney@mail.utexas.edu](mailto:kakinney@mail.utexas.edu) or Halil Berberoglu [berberoglu@me.utexas.edu](mailto:berberoglu@me.utexas.edu)

The rising demand for energy and global warming concerns are driving the search for renewable energy alternatives. Many of these alternatives require significant consumption of water or have major impacts on land utilization. In addition, fresh water resources are currently under stress. The development of renewable energy sources must address the potential environmental impacts and natural resource demands. The goal of this symposium is to promote discussions of environmentally responsible development of renewable energy sources so as to preserve our limited water resources. Topics of interest include all forms of renewable energy including solar, geothermal, hydro, biofuels and wind with an emphasis on the intersection of renewable energy production and direct and indirect impacts on natural resources.

**Spectroscopic Investigations of Metal Interactions at Mineral/Water/Microbial Interfaces** For more information contact Christopher S. Kim, Chapman University, 714-628-7363, [cskim@chapman.edu](mailto:cskim@chapman.edu) or Colleen Hansel, [hansel@deas.harvard.edu](mailto:hansel@deas.harvard.edu)

Geochemical reactions involving the redox, immobilization, and sequestration of metals are of primary interest when addressing issues of metal contamination and remediation in natural systems. Furthermore, the vast majority of these reactions are known to take place at the interfacial regions between minerals and water, microbes and water, and minerals and microbes. Spectroscopic methods, particularly those that utilize high intensity synchrotron-based X-rays, have proven a sophisticated tool for probing the atomic-level interactions between metals and these interfaces, providing unprecedented detail and insight into geochemical reaction mechanisms. This symposium welcomes papers that utilize spectroscopic techniques to explore reactions between metals, minerals, and/or microbes. Topics of interest include but are not limited to microbially-induced redox effects, sorption and (co)-precipitation reactions with minerals, and the surface-sensitive characterization of metals at biofilm/mineral interfaces. Both invited and contributed papers are planned.

**Future Prospects in Synchrotron x-ray Fluorescence Microprobe Analysis.** For more information contact Jay Brandes, Associate Professor Skidaway Institute of Oceanography, Savannah, (912) 598-2361, [jay.brandes@skio.usg.edu](mailto:jay.brandes@skio.usg.edu)

Many of the most pressing scientific questions of high societal impact require characterization of elemental abundances and speciation in minute samples that are heterogeneous at the sub-micrometer scale. Synchrotron radiation sources are ideal for developing high-intensity, highly-focused x-ray fluorescence probes for these types of

studies and rapid technical advances worldwide will soon provide scientists with the next generation of instruments with unprecedented spatial resolution and sensitivity. In particular, the design and construction of new low emittance-high brightness synchrotron x-ray sources and improvements in the quality and efficiency of x-ray focusing optics will allow these new instruments to routinely achieve spatial resolutions less than 200 nm with detection sensitivities for trace and major element analysis at least 50 times better than is currently available. Some instruments are striving for spatial resolutions of only a few nanometers with transition metal detection sensitivity as low as a few atoms. The newest generation of x-ray microprobes increasingly are utilizing tomographic techniques to provide users a three dimensional visualization of metal distributions in materials. The x-ray absorption spectroscopy capabilities of these instruments are also allowing scientists to evaluate elemental speciation in materials at increasingly lower abundance.

This workshop will bring together instrument designers and an interdisciplinary group of users to both allow the user community to familiarize itself with what new facilities will be available and so that instrument developers can better understand how scientists will be utilizing these molecular level probes in their future research. A number of scientific areas are impacted by the technical developments of these instruments and we hope to highlight the incredible breadth of chemical sciences where users are conducting research. Some examples include (but are not restricted to):

- Fate and Health Hazards of Contaminated Materials in the Environment
- Processes at the Interfaces between Minerals and Micro-organisms
- Global Effects of Particulates and Organisms in the Atmosphere and Oceans
- Chemical Evolution of Our Solar System
- Metal Homeostasis and Ionomics
- Essential Metals in Cells and Organisms and in Disease Mechanisms
- Metals as Therapies and in Medical Imaging and Diagnostics
- Catalysis and Chemical processes on the Single Particle Scale
- Elemental partitioning in microelectronics
- Elemental diffusion into microcrystalline domains

**The Need for Eclecticism in Modeling Adsorption at Mineral/Water Interfaces** Co-sponsored by the Environmental Chemistry and Colloid & Surface Chemistry Divisions. For more information contact Juan Antelo, University of Santiago de Compostela, Spain, Physical Chemistry Department, [juan.antelo@usc.es](mailto:juan.antelo@usc.es). Marcelo Avena, Universidad Nacional del Sur, Bahía Blanca, Argentina, Chemistry Department, [mavena@uns.edu.ar](mailto:mavena@uns.edu.ar). Mario Villalobos, UNAM, Mexico City, Environmental Bio-Geochemistry Group, [mar.villa@stanfordalumni.org](mailto:mar.villa@stanfordalumni.org).

The biogeochemical cycles of most elements and chemical species of environmental relevance show a significant contribution from adsorption processes to mineral surfaces. The accurate description of the adsorption behavior of aqueous species in relation to pH, ionic strength, and competition with other adsorbates on relevant mineral surfaces is of utmost importance to ultimately predict their mobility and transport. We have come a long way since application of semi-empirical models, such as the Freundlich and Langmuir adsorption isotherm, and a suite of more thermodynamically-based Surface Complexation Models (SCM's) has been developed to date.

SCM's may now be adequately constrained more consistently with the wealth of spectroscopic information available and ever growing knowledge on structural surface details. However, the complexity of the bio/geochemical systems whose behavior these models strive to describe still poses considerable challenges, especially in being at once true to reality and in taking into account all important factors involved, sometimes even for simple binary systems.

We invite contributions on modeling investigations of adsorption processes occurring at mineral/water interfaces of geochemical and biogeochemical relevance, including bacterial cell/water interfaces. Especially welcome are those modeling efforts that involve conceptual approaches including multiple tools and/or theories, and those that in addition to describing experimental adsorption behavior provide complementary insight into the microscopic and molecular interactions and mechanisms involved. We also encourage papers on adsorption modeling of actual geochemical or biogeochemical systems, or those that approach their complexity, including semi-empirical modeling

efforts that provide highly practical applications to describe transport as well. Molecular modeling efforts, thermodynamic investigations, and structurally-based models of nanoparticulate minerals that advance knowledge of adsorption behavior at the mineral/water interface will also be considered.

Confirmed invited speakers include: Dimitri Sverjensky (Johns Hopkins University), Sabine Goldberg (US Salinity Lab), Nikola Kallay (University of Zagreb), Barry Bickmore (Brigham Young University), Moira Ridley (Texas Tech University), Douglas Kent (US Geological Survey), Tjisse Hiemstra (Wageningen University).

**General Geochemistry (Oral and Posters).** For more information: Lynn Katz, [lynnkatz@mail.utexas.edu](mailto:lynnkatz@mail.utexas.edu).

**Undergraduate Research Posters.** The Geochemistry Division is seeking participation of undergraduate students in the ACS symposia. Awards are available for high-quality posters. This is a great opportunity to meet faculty from across the nation and discuss career and graduate school possibilities. Submit your poster abstract (only 150 words) to the General Geochemistry Session or to any of the symposia listed above. For more information: Lynn Katz, University of Texas, [lynnkatz@mail.utexas.edu](mailto:lynnkatz@mail.utexas.edu)

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