



GEOC



ACS Geochemistry Division Newsletter

Fall 2013

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The 246th ACS National Meeting

Indianapolis, IN
September 8-12 2013

Geochemistry Sessions

Biogeochemical controls on transition metal concentrations in natural waters

Because transition and post-transition metals in natural waters can serve as productivity-limiting micronutrients or as toxins, the processes that govern concentration, distribution, and/or speciation of these elements are of critical importance in a wide range of geochemical contexts. These processes include, but are not limited to, biological consumption, reactions at mineral surfaces, organic complexation, redox reactions, and sediment diagenesis. This session will present recent studies in natural, experimental, and computational systems aiming to elucidate past and

present relationships between metal chemistry of natural waters, biological use of transition metals, abiotic reactions affecting trace metals, and geochemistry of marine and terrestrial sediments that record evolution of these relationships over geological time.

Organizers: Laura Wasylenki (lauraw@indiana.edu) and Lev Spivak-Birndorf (lspivakb@indiana.edu) of Indiana University.

Chemical approaches to understanding metabolic activity of microorganisms in environmental settings through geological time.

Microorganisms exert a significant control on a number of element cycles in environments past and present largely through metabolism.

A detailed look at metabolic processes requires linking the geochemistry of an environmental system with investigation of specific biochemical reactions being utilized by microorganisms. In essence, the chemistry inside the cell is tied to the chemistry outside the cell.

Characterizing the geochemical setting outside a cell requires understanding chemical details (aqueous speciation, mineralogy, cell-mineral-water interactions, symbiosis between microbial communities) at the appropriate scale (single cell to community niches to larger spatial relationships). Understand cellular chemistry requires detection of the detailed biochemistry each cell may be employing (genomic, proteomic, enzyme based analyses) in both controlled lab and field settings. This session seeks to bring together researchers investigating detailed chemistry both inside and outside microbial cells towards understanding how microbial metabolisms interact

with different environments using a variety of approaches.

Conveners: Greg Druschel, Kevin Mandernack, EJ Crane, Lisa Pratt

Geochemistry of Shales: From Gas to Hydraulic Fracturing

Owing to the rising global demand for, and consumption of hydrocarbon-based products, the interest in unconventional resources such as shale gas has been increasing. In the United States, gas production from shales has increased from 0.39 TCF in 2000 to 4.80 TCF in 2010 and currently accounts for more than 20 percent of the total U.S. natural gas production. Interest in hydrocarbons from unconventional tight shale reservoirs has grown in other countries as well. The current focus on worldwide shale gas exploration and extraction necessitates a better understanding of the source rock/reservoir

GEOC: Division of Geochemistry	S	M	T	W	T
Geochemistry of Shales: From Gas to Hydraulic Fracturing**		A			
Biogeochemical Controls on Transition Metal Concentrations in Natural Waters**		P			
Sci-Mix		E			
Kinetics of Mineral Growth and Dissolution from the Nanoscale to the Macroscale			A		
Chemical Approaches to Understanding Metabolic Activity of Microorganisms in Environmental Settings through Geological Time**			P		
Kinetics of Geochemical and Microbial Reactions in Aqueous Systems			P		
Co-sponsored Symposia:					
Selecting a co-sponsored symposia will take you outside of the current Committee, Secretariat or Division					
Biogeochemical Interactions Affecting Bioavailability and Remediation of Hazardous Substances in the Environment*(ENVR)	D	A		E	
Environmental Fate and Reactivity of Highly Condensed Aromatic Carbon*(ENVR)	D			E	
Environmental Implications and Effects of Unconventional Gas Development*(ENVR)				AE	
Fate of Environmental Pollutants in Biogeochemical Interfaces*(ENVR)				E	A

Legend

A = AM; **P** = PM; **D** = AM/PM; **E** = EVE;

AE = AM/EVE; **DE** = AM/PM/EVE; **PE** = PM/EVE;

*Cosponsored symposium with primary organizer shown in parenthesis; located with primary organizer.

**Primary organizer of cosponsored symposium.

characteristics of shale gas formations as well as the environmental consequences of shale gas development.

This symposium will focus on the geochemistry of gas shales. We invite the submission of papers on various aspects of the geochemistry of shales and shale gas, as well as the geochemical issues related to gas extraction, such as fracture stimulation and its environmental implications.

Organizers: Maria Mastalerz (mmastale@indiana.edu) and Nancy R. Hasenmueller (hasenmue@indiana.edu), Indiana Geological Survey, Indiana University, 611 North Walnut Grove Avenue, Bloomington, IN 47405-2208

Kinetics of geochemical and microbial reactions in aqueous systems

The kinetics of geochemical and microbial reactions in aqueous systems has to be considered to better describe biogeochemical processes in fresh and marine waters in low or high temperature conditions. Redox reactions, gas diffusion and reactions, isotopic fractionations, water-rock interactions, and microbial processes often cannot be assessed using an equilibrium approach. In addition, rates of specific processes measured in the natural environment often are not comparable to existing kinetic rate laws derived from laboratory experiments. This session seeks to illustrate several approaches to describing geochemical and microbial kinetics in field and/or laboratory environments. We encourage submissions based on any combination of field, lab, and/or

theoretical treatment of kinetic parameters, and their eventual application to describe important processes in fresh and marine waters. This session is organized by Greg Druschel (gdrusche@iupui.edu), Bill Gilhooly (wgilhool@iupui.edu) and Martial Taillefert (mtaillef@eas.gatech.edu).

Kinetics of Mineral Growth and Dissolution from the Nanoscale to the Macroscale

Understanding the growth and dissolution of minerals is of critical importance in order to quantitatively predict rates and reactions at a variety of scales, such as including rates derived from laboratory experiments in reactive transport models. Growth and dissolution of minerals are controlled by a variety of factors, that can change across the orders of magnitude differences in these spatiotemporal scales. For instance, at the nanoscale, growth and dissolution is controlled by ion (or other molecular species) attachment to and detachment from the surface, however accurately including these reactions into large-scale models is a major challenge. Other distinct processes affect growth and dissolution at the pore scale and larger, such as pore-size volume, fluid flow, and surface roughness will need to be included in reactive reactive transport simulations. This session aims to highlight recent experimental and computational work



the Indiana War Memorial Plaza

on the kinetics of reactions occurring on mineral surfaces, including studies at the nanoscale, the pore scale, and the macroscale. We are also particularly interested in research that bridges these spatiotemporal scales. This session is organized by Man Xu, Jacquelyn Bracco, Andrew Stack, and Steven Higgins.

General Poster Session

This is a general poster session for the Geochemistry Division/SCI-MIX.

Business Meeting

Tuesday 9/10
5:00 PM

Indiana Convention
Center Room 142

Refreshments and
hors-d'oeuvres
served!

ABOUT US



The American Chemical Society

The ACS is the world's largest scientific society and one of the world's leading sources of authoritative scientific information. A nonprofit organization, chartered by Congress, ACS is at the forefront of the evolving worldwide chemical enterprise and the premier professional home for chemists, chemical engineers and related professions around the globe.

For more information:
ACS.org



The Geochemistry Division

The purpose of the Geochemistry division is to advance the study of geochemistry. Members of our division study a wide range of topics including, but not limited to, biogeochemistry, isotope geochemistry, interfacial geochemistry, cosmochemistry, petroleum geochemistry, computational geochemistry, and microbial geochemistry.

The goals of the division are:

1. To encourage the highest standards of excellence in developing and applying chemistry and related sciences as they pertain to the understanding and exploration of the Earth's geosphere and that of extraterrestrial bodies.
2. To promote the development of geochemical science in both academic institutions and in industry.
3. To improve the qualifications and usefulness of geochemists through high standards of professional ethics, education, and attainment.

For more information:
geochemistrydivision.
sites.acs.org

Spring 2014 ACS National Meeting

Dallas, TX: March 16-20
Abstracts due 10/7!

Sessions include Modeling the interface: mineralogy, environment and energy applications

Organizers: Paolo Raiteri, Andrey Kalinichev, Peter Zapol, Stephen Parker

Geochemical Processes at Mineral-Water Interfaces: From Atomic-Scale Observations to Field-Scale Phenomena (see page 11)

Organizers: Francesco Bellucci, Anastasia G. Ilgen, Sebastien Kerisit, Sang Soo Lee

Geochemistry of Nuclear Waste Storage and Disposition

Organizers: Eric M. Pierce, Louise J. Criscenti, and Joseph V. Ryan

Geochemistry and Reactive Transport in Shale Nanopores

Organizers: Louise Criscenti, Thomas Dewers, Young-Shin Jun, Yifeng Wang, Hongkyu Yoon

Advances in understanding the environmental geochemistry of manganese (Mn) oxides

Organizers: Xionghan Feng, Wei Li, Mengqiang Zhu

Don't forget about the **Geochemistry Poster Session**

Organizer: Andrew Stack

Dr. David Dixon recently elected ACS fellow!



Join us in congratulating Dr. David A. Dixon, the Robert Ramsay Professor of Chemistry at the University of Alabama for being the first member of the Geochemistry Division to be named an ACS Fellow.

This award recognizes outstanding achievements in, and contributions to science, the profession, and the American Chemical Society that was first created in 2009.

Dr. Dixon's main research applies numerical techniques for the simulation of chemical problems with a focus on fluorine and aqueous metal ion chemistry. He has applied computational methods to solve environmental problems, specifically those facing the Department of Energy (DOE) nuclear weapons production complex.

Areas of research emphasis include computational catalysis, fluorine chemistry, computational thermochemistry and kinetics, relativistic effects in quantum chemistry for actinide chemistry, prediction of NMR chemical shifts especially for fluorinated materials, solid state chemistry, aqueous metal ion chemistry for geochemical applications, the design of new separations materials including force field development, and new developments in density functional theory.

Dr. Dixon has served as chairman of the ACS Division of Fluorine Chemistry, ACS councilor, chair of the 20th Winter Fluorine Conference, and as a member of the executive committee of the division.

He is also on the editorial advisory board of the Journal of Physical Chemistry. He was awarded the 2003 ACS Award for Creative Work in Fluorine Chemistry and is a Fellow of the American Association for the Advancement of Science and the American Physical Society.

He also received the DOE Hydrogen Program R&D Award for Outstanding Contributions to Hydrogen Storage Technologies.

He has been a member of the Geochemistry Division since 2004.

The 2013 The ACS Geochemistry Division Medal

The 2013 Geochemistry Division Medal was awarded to Dr. George W. Luther III, Professor of Oceanography, University of Delaware, for his wide-ranging fundamental contributions to aqueous geochemistry.



These contributions include application of physical inorganic chemistry to understanding electron transfer in natural waters; development of chemical sensors and the application of voltammetry to quantifying trace element speciation in natural waters; and elucidation of chemical and microbial processes in metal and sulfur cycling.

Dr. Luther has been heavily involved in the Geochemistry Division of the ACS since

1985, including as Chair of the Division and councilor for more than 10 years. He has also occupied diverse positions across the ACS, including in other divisions and for the local and national chapters of the ACS.

He is the editor in chief of Aquatic Geochemistry and an associate editor of Marine Chemistry and Frontiers in Microbiological Chemistry. His scientific achievements have been recently recognized nationally: he was named a Fellow for the American Geophysical Union in 2012 and the American Association for the Advancement of Science in 2011. He was also the recipient of the Geochemical Society's Claire C. Patterson Award in 2004.

Besides his scientific achievements, Dr. Luther has been heavily involved in the Oceanographic Community, either as a member of the steering committees of FOCUS (the future of Chemical Oceanography in the US), ORION (the Ocean Research Interactive Observatory Network), and RIDGE 2000, or as a committee member of TOS (The Oceanography Society), DESSC (DEep Submergence Science

Committee), RHOC (Replacement Human Occupied vehicle oversight Committee), and InterRidge-SCOR (International Cooperation in Ridge Crests-Scientific Committee on Oceanographic Research).

The ACS Geochemistry Division Medal was awarded at a special Geochemistry Division awards symposium, which was held at the ACS National Meeting in New Orleans, LA: 7-11 April 2013.

As part of the symposium, talks were given by a wide range of members.

After the presentation of the award, Dr. Luther's contributions were celebrated with a series of invited lectures highlighting critical issues in aqueous biogeochemistry.



Frank Millero presenting George Luther with the 2013 Geochemistry Medal.



Alison Butler giving a talk on bio(geo)inorganic chemistry of marine environments



Dave Rickard giving a talk on nucleation kinetics and iron sulfide formation.



Brad Tebo giving a talk on the bioinorganic mechanisms of manganese oxidation during the Medal Symposium.

The Program Chair Elect: Dr. Sebastien Kerisit



Sebastien Kerisit is a research scientist at the Pacific Northwest National Laboratory. Sebastien received his PhD in

computational chemistry from the University of Bath, United Kingdom.

His research interests cover a range of topics relevant to the geochemistry community and include the chemistry of mineral-water interfaces, carbon capture and sequestration, the aqueous corrosion of glasses, the mechanisms of mineral nucleation and growth, and the redox properties of natural systems.

His primary expertise is in the development and application of atomistic and molecular simulation techniques for modeling the structure and reactivity of solids and their interfaces.

Sebastien has attended ACS National Meetings since 2003, became an ACS member in 2006, and has organized and chaired several symposia at National Meetings over the last few years.

He also frequently serves as a reviewer for ACS journals and serves on the Editorial Board of *Geochemical Transactions*, the official journal of the Geochemistry Division.



Brief Q&A With Dr. Sebastien Kerisit

Give us a quick sense of your journey to get to where you are?

I grew up in sunny southern France but left for rainy Bath in England for my undergraduate and postgraduate studies. I have always enjoyed the physical sciences but I started to develop a passion for chemistry during my first year in England; maybe because, being in a foreign country, the lectures were the only thing I could understand! Upon finishing my PhD with Prof. Steve Parker in 2004, I left England to take a postdoctoral position at PNNL in Washington State working with Dr. Kevin Rosso. I was hired as a research scientist in the Geochemistry Group two years later and I have been there since. I feel very fortunate to have had exceptional mentors throughout this journey.

What aspect of your research are you most excited about today?

Although I am primarily a computational chemist, I have recently begun to lead a new combined computational-experimental research program on heteroepitaxial nucleation and growth at mineral-water interfaces. Together with Dr. Man Xu and several colleagues at PNNL, we are using a range of experimental techniques to unravel complex interfacial mechanisms. Having always worked with computer simulations, designing experiments and analyzing experimental data is new and exciting to me. We are also fortunate to have access to state-of-the-art capabilities through the Environmental Molecular Sciences Laboratory at PNNL. Correlating information from all these techniques makes for a fascinating puzzle to solve as well as some late nights at the office!

Where do you see the Geochemistry Division headed in the next few years?

I see the Geochemistry Division growing significantly over the next few years as more scientific research becomes directed at geochemistry-related topics. An increasing number of issues at the forefront of public attention would benefit from an improved understanding of geochemical systems and, as the discussion of our societies' geological impact grows, we can expect more students to be drawn to geochemical sciences.

Member Profiles

Your chance to meet some of the students and members who help run the geochemistry division behind the scenes

Anastasia Ilgen



My current research interests center on trace metal(oid) fate and transport in soil and aqueous environments, with a focus on mineral-water interface chemistry. I received my Ph.D. in Environmental Chemistry from the University of Alaska Fairbanks (UAF) in 2010, which I completed while working under the supervision of Prof. Tom Trainor. My dissertation was on the chemical forms and heterogeneous redox reactions of arsenic (As) and antimony (Sb) at the clay mineral-water interface. During my postdoctoral employment at UAF (2011/12), I worked on the redox chemistry of metallic antimony, which has direct relevance to the fate and transport of antimony within contaminated military shooting range soils. I obtained my Specialist Diploma (equivalent to MS/MSc) with highest honors in Water Resources Engineering at Kamchatka State Technical University, Petropavlovsk-Kamchatsky, Russia.

In September 2012, I started as a senior member of technical staff at the Geochemistry Department, Sandia National Laboratories, Albuquerque, NM. I love working in a national laboratory setting, and am participating in a variety of projects while continuing my earlier research in clay mineral surface chemistry. Another project in which I am participating is part of a large EFRC (Energy Frontier Research Center) effort, and I am working on the geochemical modeling of interactions between CO₂ and saline aquifer. An additional project is examining the geochemical changes within Arctic soils in response to the degradation of permafrost due to climate change.

I enjoy field work, and getting my hands dirty both in the field and doing laboratory experiments, and also get really excited about data analysis and modeling. I'm addicted to that rush you get when you solve a problem or see something new. I can't think of anything I'd rather be doing than geochemistry!

I've been a member of the ACS Geochemistry Division since 2008. Louise Criscenti has passed on the membership chair duties to me this year, and it has been great contributing to the community this way. We are also organizing one of the GEOC sessions for the Spring 2014 ACS meeting: **Geochemical Processes at Mineral-Water Interfaces: From Atomic-Scale Observations to Field-Scale Phenomena (see page 11)**.

News Update

One of the main beamline geoscientists use – GSECARS at Argonne National Lab - has recently been updated doubling the amount of undulator beam time available to users starting last January!

Check out the full story at <http://gsecars.uchicago.edu/news/gsecars-completes-canted-undulator-upgrade>

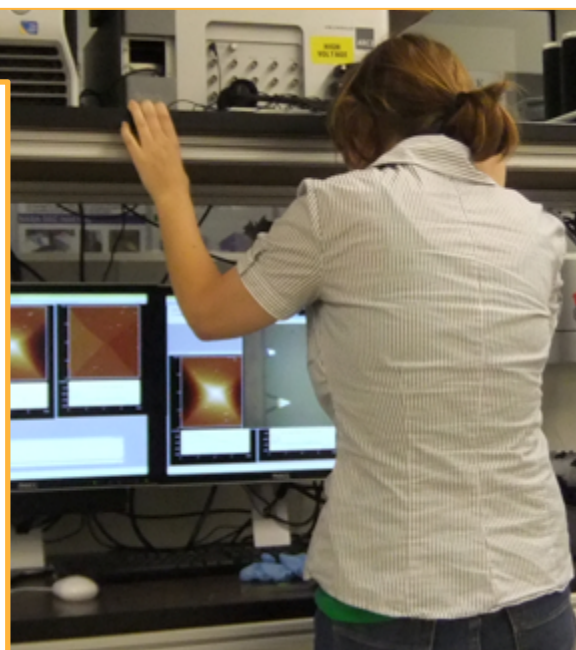
Jacquelyn Bracco

I am a 2nd year PhD student at Wright State University with Prof. Steve Higgins. In my research I study the growth of carbonate minerals using atomic force microscopy (AFM). We are also working on developing an AFM that can operate at higher temperatures. I'm really excited about building a new AFM as it's something a bit different than what I've been working on in the past. It's forcing me to learn a whole new set of skills as it is posing some interesting challenges.

I started doing research with Dr. Andrew Stack as an undergrad at Georgia Tech and stayed for my masters. During my masters, he left to take a job at Oak Ridge and brought me with him to finish up my research for that degree. Since he knew I was interested in instrumentation, he suggested I go work with Dr. Higgins for my PhD.

I was first drawn to my field when I realized I really enjoyed the mineralogy parts of a geochemistry class I took as an undergrad. In the future, I would like to work either in a national laboratory setting or in industry after I graduate, preferably doing research in a laboratory setting.

I'm serving now as the assistant webmaster to the geochemistry division, so let me know if there is anything you want to see in the website.



Liz Percak-Dennett



I am a PhD Candidate at the University of Wisconsin-Madison studying microbial Fe oxidation at circumneutral pH with Dr. Eric Roden. I completed my MS at Wisconsin examining Fe isotope fractionation in simulated ancient Earth environments with both Dr. Roden and Dr. Clark Johnson. My undergraduate degree was from the University of Alaska Anchorage where I worked with Dr. LeeAnn Munk, and this is where I first fell in love with low-temperature geochemistry.

Graduate school has enabled me to develop as a member of the greater scientific community while allowing me the opportunity to develop a diverse skill set of microbiology and geochemical techniques.

One of my main passions is science outreach and communication: I love the challenge of breaking down complex ideas into tangible pieces that everyone can understand. Plus, sharing the value of the work we do to the public at large is, in my opinion, a key component in insuring the future of science.

My favorite element is carbon, because without it there would be no life (at least that we know of), but iron is a close second. I love iron to much, in fact, that I was Fe for Halloween last year, and will be soon completing my first Ironman triathlon.

Dear Geochemistry Division,

Many thanks for voting in our elections last December: **Sebastien Kerisit** has been elected our new Program Chair-Elect. **Lee Penn** is our ACS Councilor. Sebastien will be Program Chair-elect for calendar year 2013, Program Chair in 2014, Division Chair in 2015, and Past Chair in 2016. Lee will be ACS Councilor for three years, through 2015. Also **Andrew Bishop** is taking on the role of Extended Programming Coordinator and will be involved in both long range programming at national meetings and initiating selective programming at regional meetings.

Congratulations to Sebastien and Lee, and a big thanks for everyone who ran for office! Here is the Geochemistry's divisions executive committee:

Division Chair:	Martial Taillefert, mtaillef@eas.gatech.edu
Past Division Chair:	Lee Penn, rleepenn@umn.edu
Program Chair:	Andrew Stack, stackag@ornl.gov
Program Chair-elect:	Sebastien Kerisit, sebastien.kerisit@pnnl.gov
Secretary:	Louise Criscenti, ljcrisc@sandia.gov
Treasurer:	Chris Kim, cskim@chapman.edu
ACS Councilor:	Lee Penn, rleepenn@umn.edu
Alternate Councilor:	Yoko Furukawa, yoko.furukawa@nrlssc.navy.mil
Newsletter Editor:	Liz Percak-Dennett, percakdennett@wisc.edu Johnson Olanrewaju, Olanrewa001@gannon.edu
Webmaster:	Steven R. Higgins, steven.higgins@wright.edu Jacquelyn Bracco, bracco.2@wright.edu
Extended Programming Coordinator:	Andrew Bishop, Andrew.Bishop@shell.com

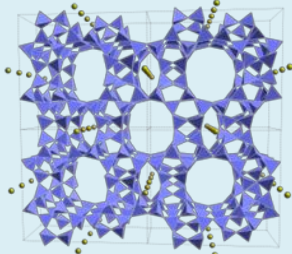
If you're interested in becoming more involved in the ACS Geochemistry Division, please consider organizing a symposium, joining a planning committee, or nominating yourself for an elected position. Any of the GEOC officers would be happy to give you more information, or discuss their work with you.

ACS Geochemistry Division Secretary, Louise J. Criscenti

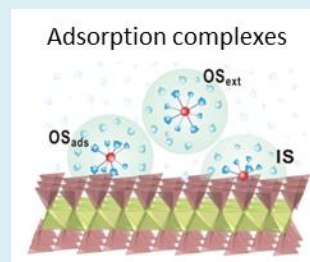
Welcome new members! Emmanuel Aluola, Enrica Balboni, Ernesto Ballester, Udo Becker, M Bellis, Ethan Black, Maik Blakely, Jacquelyn Bracco, Tari Briggs, Dale Bryant, Kevin Caple, William Casey, Jose Cerrato, Clara Chan, Gordon Chiu, Mark Colman, Allison Dammeyer, Karin Danielsson, Thomas Darrah, Fabiana Figueira, Shannon Flynn, Deliana Gabeva, Mariam Georges, Christy Gibson, Vanda Glezakou, Karen Goldenberg, Christopher Gorski, Nicole Grant, Marie Hammerstrom, Seunghee Han, Parker Hein, Yongseok Hong, Chad Jafvert, Deb Jaisi, Noemie Janot, Corinne Kuebler, Laura Lapham, Brent Lewis, Sierra Lewis, Hui Lin, Paul Lipton, Nathaniel Lyons, Marty Marin, Besty McCall, Shawn McElmurry, James McNutt, Tarek Melki, Carmine Milo, Darryl Mott, David Moyer, Satish Mynen, Ryan Nell, Brian Nieto, Keith O'Connor, Hem Pant, David Polya, Joseph Radler, Severiano Reodica, Peter Scott, Zhizhang Shen, Saif Eldin Siddeeg, Emily Singleton, Suzanne Smaglik, William Smith, Elizabeth Spencer, Kevin Sramek, Brian Stewart, Robin Sutka, Dimitri Sverjensky, Dave Szymanik, Melinda Tidrick, Peter Tremaine, Stephanie Trump, Bryan Unruh, David Vance, William Walker, Wendell Walters, Laura Wasylenki, Charmaine Weyer, Andrew Wozniak, Luis Eduardo Wu, Zelong Zhang, Ying Zhu.



Mordenite



247th ACS National Meeting & Exposition
March 16-20, 2014
Dallas, Texas
Geochemistry Division
Symposium on



**Geochemical Processes at Mineral-Water Interfaces:
 From Atomic-Scale Observations to Field-Scale Phenomena**

Organizers:

Francesco Bellucci

Chemical Sciences and Engineering Division, Argonne National Laboratory, fbellucci@anl.gov

Anastasia G. Ilgen

Geochemistry Department, Sandia National Laboratories, agilgen@sandia.gov

Sebastien Kerisit

Physical Sciences Division, Pacific Northwest National Laboratory, sebastien.kerisit@pnnl.gov

Sang Soo Lee

Chemical Sciences and Engineering Division, Argonne National Laboratory, sslee@anl.gov

Mineral-water interfacial chemistry exerts a significant control over the composition of natural environments. This symposium will consider research presentations that highlight recent experimental results on geochemical processes at mineral-water interfaces, including interface structure and reactivity, ion adsorption-desorption rate and mechanisms, chemical and biological controls on mineral nucleation, growth and dissolution, surface-mediated redox reactions, and the effects of organic matter and biota on surface reactivity. Presentations will be focused on fundamental studies of the mechanisms controlling surface and interfacial chemistry, as well as advances in experimental design and technical development for interrogating mineral-water interfaces.

Confirmed Invited Speakers:

Jeff Catalano, Washington University in St. Louis, USA

Paul Fenter, Argonne National Laboratory, USA

Andrew J. Friedrich, University of Wisconsin, USA

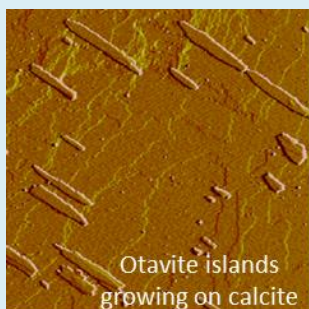
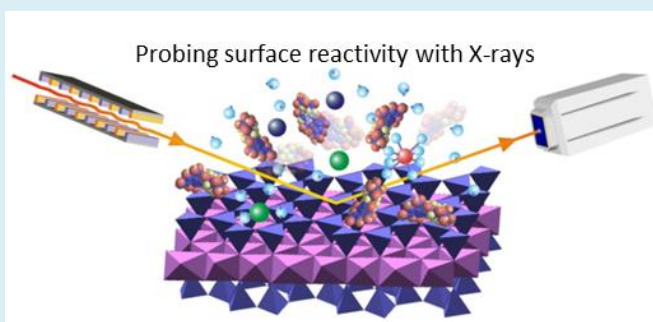
Franz Geiger, Northwestern University, USA

Lynn Katz, University of Texas, USA

Katharina Mueller, Helmholtz-Zentrum Dresden
-Rossendorf, Germany

Moritz Schmidt, Karlsruhe, Germany

Joanne Stubbs, University of Chicago, USA



Otavite islands
growing on calcite

Abstracts should be submitted on-line on the PACS abstract submission site:

<http://abstracts.acs.org>

Select GEOC and this symposium.

Follow instructions to submit a 150 word abstract.

Deadline for online abstract submission is October 7, 2013

If you have difficulty submitting an abstract, please contact the organizers.