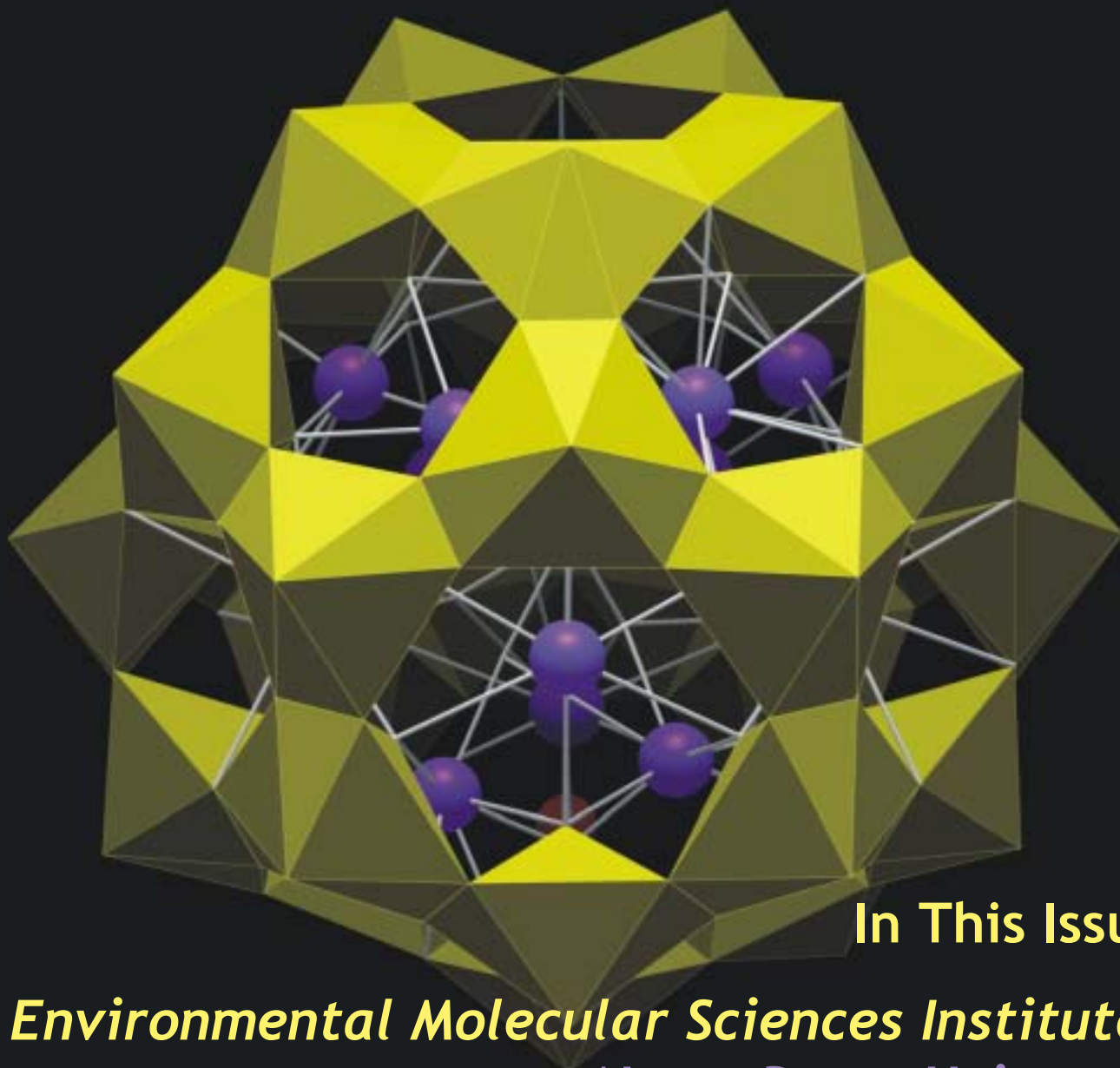


THE GEOCHEMICAL NEWS

Newsletter of The Geochemical Society
in cooperation with The European Association of Geochemistry



In This Issue:

***Environmental Molecular Sciences Institutes;
Notre Dame University
Pennsylvania State University***

January 2006
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Meet the New GS Directors



THE GEOCHEMICAL SOCIETY

The **Geochemical Society** is a nonprofit scientific society founded to encourage the application of chemistry to the solution of geological and cosmological problems. Membership is international and diverse in background, encompassing such fields as organic geochemistry, high- and low-temperature geochemistry, petrology, meteoritics, fluid-rock interaction, and isotope geochemistry. The Society produces a *Special Publications Series*, *The Geochemical News* (this quarterly newsletter), the *Reviews in Mineralogy and Geochemistry Series* (jointly with the Mineralogical Society of America), the journal *Geochimica et Cosmochimica Acta* (jointly with the Meteoritical Society), and co-publishes the electronic journal *G³* (jointly with the American Geophysical Union: AGU); grants the **V.M. Goldschmidt**, **F.W. Clarke** and **Clair C. Patterson Awards**, and, jointly with the European Association of Geochemistry (EAG), the Geochemistry Fellows title; sponsors the V.M. Goldschmidt Conference, held in North America in odd years and elsewhere in even years, jointly with the EAG; and co-sponsors the Geological Society of America annual meeting and the AGU spring meeting. The Society honors our first President, F. Earl Ingerson, and our first Goldschmidt Medalist, Paul W. Gast, with the **Ingerson** and **Gast Lectures**, held annually at the GSA Meeting and the V.M. Goldschmidt Conference, respectively. The Geochemical Society is affiliated with the American Association for the Advancement of Science and the International Union of Geological Sciences.

Members of the Organic Geochemistry Division are individuals with interests in studies on the origin, nature, geochemical significance, and behavior during diagenesis and catagenesis of naturally occurring organic substances in the Earth, and of extraterrestrial organic matter. GS members may choose to be affiliated with the OGD without any additional dues. The OGD presents the **Alfred E. Treibs Award** for major achievements in organic geochemistry, and **Best Paper** awards (student and professional) in organic geochemistry.

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THE GEOCHEMICAL NEWS

January 2006

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From the GS President,

I am happy to be writing you as the new President of the Geochemical Society. Tim Drever actually wrote me on the last day of December 2005 to "pass the torch" and so we started the New Year in a timely fashion. I am looking forward to working with all members from around the world to encourage research, education, and outreach in the field of geochemistry. The GS Officers and Directors meet at least once a year at the annual Goldschmidt meeting, and converse regularly by email to address issues concerning our Society. If you have concerns or interests, I would welcome your comments at any time.

Issues that I am looking forward to discussing in the next year include questions concerning future Goldschmidt meetings, questions concerning sub-groups of the Geochemical Society, and questions concerning how the GS might become more active in scientific outreach. I am enthusiastic to address these issues as well as others, including proposed work on our website. At this time, I would also like to welcome Marty Goldhaber as the new Vice-President and Mark McCaffrey as the newly appointed OGD Chairman. Of course, with new officers, we need to thank the "old" officers, including both Judith McKenzie who will be stepping down after six years in the presidential cycle, and Tim Drever who will now fill Judy's roll as Past President. I will particularly miss the occasional emails from Judy. We also welcome the new GS Directors, Andreas Lutge and Yaoling Niu, and bid adieu and thanks to those leaving their posts as Directors, Gilbert Hanson and Harry Elderfield.

I am looking forward to seeing many of you in Melbourne. As the first Goldschmidt "down under", the 16th Annual Goldschmidt Conference will be an event not to miss.

Susan L. Brantley, GS President



Susan Brantley

From the EAG President,

Greetings and best wishes for the New Year to EAG members everywhere. By the time that you read this, I hope that many of you will have turned your thoughts to attending this year's Goldschmidt conference in Melbourne. The key deadlines are April 13th for submission of Abstracts and June 30th for registration.

Australia presents a plethora of geochemical environments ancient and modern that have few parallels in Europe, and I hope that many of you will be able to take advantage of the impetus from attending the year's outstanding geochemical conference to see some of them. If however you find it difficult to attend conferences in such far flung locations, then you may be pleased to hear that for the foreseeable future, Goldschmidt conferences are returning to the alternation between venues in Europe and North America, with the 2007 conference in Cologne already at an advanced stage of planning.

The EAG would like to support more geochemical activities in Europe, in recognition of the very high concentration of geochemists and geochemical research that is going on in the continent. If you have ideas for meetings, workshops, conference sessions or any other activity that would promote geochemistry, please take a few minutes to get in touch with the EAG Council to see if we can help in any way.

Bruce Yardley, EAG President

Cover: Uranyl peroxide nano-cluster of composition $K_{16}(H_2O)_2(UO_2)(O_2)_2(H_2O)_2[(UO_2)(O_2)_{1.5}]_{28}^{-14}$ (Burns et al. 2005). Image credit Peter Burns.



Editors' Corner

A New Year Yet Again

2006 is underway, and Goldschmidt 2006 is coming up fast. Please send us any announcement you might have about the upcoming conference, bearing in mind that they won't be published until April. We're going to try and get the April 2006 issue out as early in the month as possible, so that any pertinent Goldschmidt announcements will reach the membership well before the abstract deadline. To do that we're going to be asking our contributors to send us material no later than March 15. That way we can have everything in place well ahead of schedule.

As always, if you're going to contribute to GN, **make sure to send all text contributions as MS Word files**, and **please DO NOT embed figures in the text file**. We absolutely cannot use any figures embedded in MS Word files, due to resolution and pixelation issues caused by transferring the data from Word to our desktop publishing software. Please **send any image files as separate, individual graphics files (GIF, JPG, TIFF formats only)**. Also, please try to send image files in as high a resolution as possible. If you have email issues sending large files, we'll be happy to instruct you where to upload files to our FTP server, or you could always publish your graphics files onto html documents that we can download on this end. If you have any other questions or concerns, please just drop us an email and we'll come up with a solution!

Until next issue,

Johnson R. Haas (johnson.haas@wmich.edu),

Carla Koretsky (carla.koretsky@wmich.edu),

Editors

2006 V. M. Goldschmidt Conference Travel Grant Program for Graduate Students Sponsored by the National Science Foundation

The Geochemical Society announces an NSF-sponsored grant program that will provide awards of up to \$1,000 to support graduate students giving talks or posters based on their own research at the 2006 Goldschmidt meeting in Melbourne, Australia. This is a competitive program and eligibility is limited to graduate candidates (Master's and Ph.D.) enrolled at accredited degree-granting institutions in the US and its territories. Applicants who wish to be considered should submit a CV, a copy of their submitted Goldschmidt abstract (with abstract number), a one page summary describing the broader impacts and significance of their research, and a budget justification (including a statement of need, detailing alternative sources of funding). Applications are encouraged from women and minority candidates. Applications will be accepted until 30 April 2006. Approximately thirty awards will be made. Please direct all enquiries to Dr. Johnson Haas, Department of Geosciences, Western Michigan University, Kalamazoo, MI 49008, USA. Tel 269-387-2878, Fax 269-387-5513, Email johnson.haas@wmich.edu. For further details see <http://www.geochemsoc.org/announce/2006goldtravel/>.

From the GS Business Office

Business Office News and Notes.

2006 looks to be a very active year for the Geochemical Society. There are many excited volunteers with excellent ideas, so be certain to stay in touch with the latest happenings on our website.

Now it is www.geochemsoc.org

Speaking of which, starting in January we have changed our web address to www.geochemsoc.org. Accordingly, the business office's address has also changed to gsoffice@geochemsoc.org. No need to fret, your bookmarks and address books to the old addresses will still work. Also with the new name we are looking into reorganizing the website. Send comments or suggestions regarding what current features you think are most useful as well as features you would like to see to the business office.

Logo Design Contest Extends Deadline

Our search for a new logo continues. Details regarding the contest can be found in this issue.

Seeking Job Announcements!

We have begun a Community Job Listing on our website, but we need your help to fill it with important job opportunities. Visit <http://www.geochemsoc.org/announce/joblist.html> to view the latest postings.

The Goldschmidt abstract deadline is fast approaching

13 April 2006 is the deadline to submit abstracts for the 2006 Melbourne Goldschmidt Conference.

For more information on abstract guidelines as well as programs, field trips, events and exhibits visit the conference website at: <http://www.goldschmidt2006.org/>

Are you interested in hosting a Goldschmidt?

The Board of Directors will be examining bids for the 2009 and 2010 Goldschmidts during the 2006 Annual Board Meeting on August 26th, in Melbourne. If you, your university and/or your city are interested in submitting a bid, please contact the GS Business Office.

Elements Production Information

- o Labels for Elements v.2 issue 1 (February 2006 - User Research Facilities in the Earth Sciences) were submitted on January 7, 2006. The issue is expected to arrive sometime in mid-February.
- o Society news materials for Elements v.2 issue 2 (April 2006 - Arsenic) were submitted in January 15, 2006. If you have any news of interest to the geochemical community or to GS members, please send it to the Business Office.
- o Future topics are as follows: June – Water on Mars, August – Early Earth, October – Glasses and Melts: Linking Geochemistry and Materials Sciences, and December – Environmental Aspects of the Nuclear Fuel Cycle.
- o For those interested in submitting a proposal for future thematic issues, please visit the Elements website at: <http://www.elementsmagazine.org/>. Click on 'Forms', then "To submit a proposal for a thematic issue".

Geochemical Society Sponsored Special Sessions at Spring AGU Meeting

The Geochemical Society is a sponsor of the 2006 Joint Assembly, 23-26 May, in Baltimore, MD. Abstracts are currently being accepted. The abstract deadline is **1 March 2006**. For more information visit <http://www.agu.org/meetings/jao6/>

Geochemical Society Sponsored Sessions

- GSo1 Geochemical Society General Contributions
- GSo2 Depleted Uranium Aerosols in the Surface Environment: Transport, Geochemical Speciation, and Implications for Human Health



Seth Davis

Presented jointly with AGU

- Uo2 Thermodynamic Variables in Magmatic and Metamorphic Processes in the Terrestrial Planets: Theoretical, Experimental and Observational Constraints
 Uo6 Atmospheric, climatic, and biological evolution at both ends of the Proterozoic Eon
 Uo7 Evolution of the Andes
 Uo8 Fluids In The Earth
 U11 Microanalysis: Small Beams, Big Science (INVITED ONLY)

Presented jointly with MSA

- Mo1 Mineralogy and the Nuclear Fuel Cycle — The 2006 Dana Symposium
 Mo3 Spectroscopy in Mineralogy: Theory and Experiment

Presented jointly with Mineral and Rock Physics

- MRo1 Mineral and Rock Physics General Contributions

Presented jointly with Microbeam Analysis Society

- MBo1 General Contributions to Microanalysis in the Earth Sciences
 MBo2 From Earth to Mars and Beyond

Presented jointly with Hydrology

- H11 Water Quality of Hydrologic Systems POSTERS
 H17 Chemical and Isotopic Tracing of Contaminated Groundwater
 H24 Scale Issues of Catchment Hydrology and Biogeochemistry

Presented jointly with Volcanology, Geochemistry, and Petrology

- Vo2 Origin, Behavior, And The Role of Magmatic Sulfur in Terrestrial Planets: Theoretical, Experimental and Observational Constraints
 Vo4 Evolution of the Early Earth
 Vo5 Tracing deep-Earth Processes With Light Elements: Insights Into the Evolution of the Crust, the Mantle and Magmas From B, Li and Be Isotope and Abundance Systematics
 Vo8 Sulfur in the Earth System: Insights Into Evolution of Surface Environments and Secrets of the Deep Earth
 Vo9 Biosignatures: Distinguishing Biology from Abiological Look-Alikes
 V10 Frontiers of Hydrothermal Geochemistry: Organic - Inorganic Interactions From Deep Crust to Volcanic Systems
 V11 Earth's Carbon Cycle: Sources, Recycling Pathways, and Geochemical Evolution

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 Marty Goldhaber, Vice-President (USGS – Denver)
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 Vincent J. Salters, Director (Florida State University)
 Yaoling Niu, Director (Durham University)
 Andreas Lutge, Director (Rice University)

2005/2006 Member Contributions to the Geochemical Society

Several members contribute to GS each year by including a contribution with their dues. If you are interested in making a donation, please contact the business office.

Contributors to the Geochemical Society

Larry K. Benninger, Peter R. Buseck, Martin M. Cassidy, William S. Courdua, Catherine E. Courriveau, Yigal Erel, Cyrus W. Field, Joris M. Gieskes, Daniel B. Hawkins, Miriam Kastner, Yousif K. Kharaka, Tadao Nishiyama, Radomir Petrovich, Michael A. Velbel

Contributors to the GS Student Travel Grant Fund

Ghislaine Crozaz, David R. Cole, Judith A. McKenzie, Paul Northrup

Contributions may be in the form of general support or may be directed toward specific programs, such as Geochemical News, the Organic Geochemistry Division, the Goldschmidt Student Travel Grant Program, the Meeting Assistance Program, Special Publications and Society Award Programs

Please Renew Your Membership!

I'll end this installment with a plea. We have truly appreciated your membership in 2005 and look forward to serving you in 2006. Please renew on-line at: http://www.geochemsoc.org/cgi-bin/gs_register_ic3.pl. Or there is a membership form in this issue which may be mailed or faxed to the business office. Remember this is your society, if you have questions about any of our programs or services, or suggestions on how to improve, please sent them to us!

Best wishes for a productive and healthy 2006,

Seth Davis

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Geochemical Society Members: Action Items

Interested in helping out your organization?
Here are some action items you can do to help!

Renew your membership!

Send information for www.geochemsoc.org

- o Job Postings
- o Announcements
- o Meetings Calendar

Send useful comments or suggestions to the business office about our activities and programs, such as:

- o Geochemical News.
- o Elements
- o www.geochemsoc.org
- o The Organic Geochemistry Division
- o The Goldschmidt Conference

Submit a design for the logo contest.

Make a Donation to the Geochemical Society.

In Memoriam: Alfred A. Levinson (1927-2005)

Dr. Alfred A. Levinson passed away at on Monday, December 12, 2005, after a long but private battle with lung cancer, at the age of 78 years.

A native of Staten Island, NY, Al served in the U.S. Navy during World War II and subsequently obtained his doctorate degree in mineralogy from the University of Michigan, Ann Arbor, in 1952. His distinguished career as a Geologist/Mineralogist included positions at Ohio State University, Dow Chemical, and Gulf Research before he joined the University of Calgary in 1967 as Professor of Geology. During his tenure at U of C, he not only taught thousands of students, but he also served on the editorial boards of several major geological journals, edited the first scientific volumes on the rocks recovered during the 1969 Apollo 11 voyage to the moon, and authored a number of books. Shortly before his retirement from U of C in 1994, Al developed an interest in gemology that he pursued as author, editor, and lecturer until his death. In 2001, a new mineral species, levinsonite, was named in his honour. Al is survived by his sisters, Florence Spungen of Riverwoods, IL and Sheila Leventhal of Palm Beach Gardens, FL; numerous nieces and nephews; and his long-time friend Alice Keller of Encinitas, CA.

A religious service was held at Temple BNai Tikva (900 47 Avenue S.W.) on Monday, December 12, 2005 at 3:30 p.m. A memorial service was held at the University of Calgary on January 21, 2006 at 3:00 PM.

Yours truly,
Carl Forman
Executor



Alfred A. Levinson

SciPodders: Podcasts for Geochemists

Podcasting is the newest form of mass media, and in less than a year has grown from an obscure avocation for techies to a major cultural phenomenon. Most of this growth has been fertilized by the amazing success of Apple's iPod personal mp3 player technology (those white wires dangling from your students' ears), which itself took off because of the popularity of mp3. Podcasting arose in 2004 from the synergy and new RSS syndication technology that made it easy to encapsulate high-quality audio content and post it on the internet. What distinguishes podcasting from earlier streaming technologies such as RealAudio is the ability to subscribe to a podcast feed, new content downloaded to your computer as soon as they are published. Unlike streaming feeds, you don't have to be connected to the internet in real time to listen to a podcast episode; episodes are stored as individual mp3 files on your local machine, and can be moved about like any other music file. It's radio as it has recently appeared, aided by the release of Apple's new video iPod, and this development is sure to foster rapid mutation of the particular medium. Nonetheless, all of the below are strictly audio feeds.

An obvious advantage of podcasting is that it democratizes the capability of broadcasting. With podcasting anyone with a computer, a microphone and access to the internet can host her own radio show – or if you prefer, mp3 for an FCC license (or your local station). Since the inception of podcasting in 2004, the number of individual podcast feeds has skyrocketed into the thousands. iTunes now hosts a convenient podcatching client with search functionality, so it's easy to find a podcast that appeals to your interests. Program quality can vary, as you might expect. But among the cacophony of tinny voices there are some very well produced, informative and entertaining feeds that focus on the natural sciences. The best of these are invaluable sources of science news that I now listen to regularly. Some focus on particular science disciplines while others offer a news potpourri of science discoveries, controversies, and current events that are worthy as 'assigned listening' for students. And all the ones I've listened to and recommend below are free to download.



Podcasting of ubiquitous iPods (and clones) technology that made it easy to encapsulate content and post it on the internet. Unlike streaming feeds, you don't have to be connected to the internet in real time to listen to a podcast episode; episodes are stored as individual mp3 files on your local machine, and can be moved about like any other music file. It's radio as it has recently appeared, aided by the release of Apple's new video iPod, and this development is sure to foster rapid mutation of the particular medium. Nonetheless, all of the below are strictly audio feeds.

podcasting is that it massively democratizes the capability of broadcasting audio content. With podcasting anyone with a computer, an internet connection, a microphone and access to a server can host her own radio magazine – without the need for an FCC license (or your local station). Since early 2005 the number of individual podcast feeds has skyrocketed into the thousands.

Science news feeds are offered by a wide variety of creators, including traditional outlets such as the major television networks, but the best podcasts have no connection to the dusty archons of mass media. Some of the most entertaining are aimed at the general public, such as the **Naked Scientists Science Radio Show** podcast (www.thenakedscientists.com), a BBC production from the UK. This is an hour-length podcast feed of the popular British radio program, and features science news headlines, eclectic interviews with notable scientists, questions from callers, and on-air science quizzes for kids of all ages. A recent broadcast featured Harry Elderfield, who discussed global climate change. Another notable British production is the **New Scientist Podcast** (www.newscientist.com/podcast.ns), which provides a weekly science news brief followed by an in-depth discussion of selected science topics, again including interviews with major figures in the respective disciplines. National Public Radio listeners in the US will be familiar with **Science Friday** (www.sciencefriday.com), the weekly segment of NPR's Talk of the Nation radio program spotlighting science current events. Science Friday offers a full hour of discussion on usually one or two major science stories. Its coverage tends toward the simplistic, and host Ira Flatow

will often interrupt guest scientists to make them explain to listeners, say, what is an atom. Aimed at a US audience, this program will also sometimes resort to the fatuous 'both sides' dynamic where one guest will be invited to discuss the global scientific consensus of some issue, and the producers will dig up a second guest to represent 'the other side' viewpoint held by some peculiar faction of ideologues or paid shills whose terse membership list stretches to absurdity the concept of 'minority opinion'. Still, it's an interesting show and it uses small words.

On the more humorous end of the scale is **This Week in Science** (www.twis.org), a radio show and podcast produced by the University of California at Davis and hosted by a neuroscience Ph.D. student and a layman kibitzer. Also an hour-long show, TWIS provides science news headlines, interviews with notable investigators, and other sci-miscellany from an irreverent perspective. It's actually a very funny show, and one of my favorites for casual listening. Hosted by student-types (if I may be forgiven a prejudicial inference) this show is very accessible and doesn't talk down to its listeners.

In addition to the many general science-news podcasts, a wide spectrum of specialty programs has sprung up in the last few months. I can't keep up with all of them, and an exhaustive discussion is beyond me, but I've found a few notable examples that touch on the earth sciences and geochemistry. **MicrobeWorld Radio** (www.microbeworld.org) is sponsored by the American Society for Microbiology, and offers 90 second news briefs that each focus on a current item in microbial current events. **NASA's Jet Propulsion Laboratory Podcast** (www.jpl.nasa.gov) publishes brief headline articles on the latest events in space exploration. The podcast of **Planetquest – The Search for Another Earth** (planetquest.jpl.nasa.gov/index.cfm) provides news from the world of astronomers who hunt for extrasolar planets, although episodes for this feed are sparse. **Universe Today** (www.universetoday.com) follows the science news format of many other podcasts, but focuses on current events and new discoveries from astronomy, astrobiology, and planetary science. Another source of astronomy and planetary science news can be found at the **W. M. Keck Observatory** podcast (www.keckobservatory.org/news/education/mp3.php). A new podcast feed from the **University of Bath – Public Lectures** (feed://www.bath.ac.uk/podcast/public-lectures-podcast.xml) promises both first rate science lectures from giants in their fields, and also one of the world's longest podcast URL addresses. Only one episode of the Bath podcast is yet available, but more are sure to come.

One of my favorite science-related podcasts is **Skepticality** (www.skepticality.com). Hosts Derek and Swoopy discuss pseudoscience, the paranormal, and other manifestations of nonsense that could use a strong dose of skeptical scientific thinking. The relevance to earth science topics is obvious, and many of their shows discuss the apparently deathless debate over evolution in the US, global climate change, astronomy, and other areas where science is under fire from the epsilons. If you're a fan of well-known pseudoscience debunker The Amazing Randi, you'll love this program. Host Derek Colanduno is currently recovering from a near-fatal brain aneurysm he suffered last fall, and so the show has been on quasi-hiatus for the last several months. Nonetheless, you can download all of last year's episodes through the subscription feed. Right now Derek is on the mend, and new episodes are sure to be coming soon. My hopes are for his speedy recovery.

Most science podcasts are journalistic, but already a few professors around the world (mostly in the US and Britain) have begun to publish their class lectures as podcasts. This is an intriguing new format for delivery of knowledge to students and to the public, but it remains to be seen if many academics will adopt the strategy. No doubt many of us would fear that if our lectures were online our classrooms would be empty. And perhaps so. I'll let you know, if I ever try it.

In summary, podcasts are an easy, convenient and very enjoyable way to access exciting science news and viewpoints from around the world. Right now the majority of science podcasts are not discipline-specific, but rather discuss any and all developments in the 'sciences', usually dominated by medical or technological topics. Among the natural sciences astronomy has a clear lead in coverage, but only time will tell if that will remain the case. Right now there is a clear paucity of dedicated earth science podcasts, and to my knowledge no podcasts focus on non-fossil geology or geochemistry. That's unfortunate, and perhaps one of us will one day step forward to fill that gap. I'll be listening.

Johnson R. Haas
Western Michigan University



Do you dig rocks and love life?

Biogeosciences.org is an innovative Web site bridging the earth and life sciences. It provides a single resource for all things biogeoscience related. Released in June 2004, the site has continued to grow and expand, becoming a natural home for biogeoscience discussion, resources, and promotion.

Biogeosciences.org is a non-commercial Web site developed by the Geological Society of America (GSA) and its partnered professional societies. These partnered societies, which include the Geochemical Society, are a constant supply of up to date information and resources. Biogeosciences.org is supported by a grant from the Biogeosciences program of the National Science Foundation.

The site offers biogeoscience links and program resources for kids, students, undergraduates, and teachers. There is frequently updated information on job openings, funding opportunities, and degree programs. There are interviews with people working in the biogeosciences and links to useful publications and articles. The site also contains a calendar of biogeoscience related meetings, fieldtrips, workshops and symposia from around the world.

Biogeosciences.org also offers an interactive component. Through the site people are able to submit material that they think would be of interest to the biogeosciences community, or add their names and research interests to a growing list of biogeoscientists. One of the most exciting and interactive features on biogeosciences.org is the discussion forum, which allows for the rapid sharing of ideas and opinions, as well as an opportunity to ask questions of a large community of scientists. Yet another interactive feature is an image gallery where pictures are exchanged freely for educational purposes.

Interested parties are encouraged to visit the Web site. Any inquires (including submission of material for posting) should be directed to Sarah Leibson (web@biogeosciences.org), Web Site Coordinator, Biogeosciences.org.



Meet the New 2006 GS Directors

Martin Goldhaber received his BS in Chemistry (1968) and PhD in Geochemistry (1973) both from UCLA. After spending a year as a Post Doc at Yale he joined the USGS in 1975. He is currently a Senior Scientist at the USGS where he received the Department of the Interior Meritorious Service Award and recently served a term as the Chief Scientist for Geology. Marty has been a member of the Geochemical Society since 1972 and has been involved in the Society in a number of roles; most recently as Program Chair. He is a fellow of the Geological Society of America and the Society of Economic Geologists. Marty has served on the editorial boards of *Economic Geology*, *American Journal of Science*, and *Geochimica* (two terms) and has served on advisory boards for the Geological Society of America, the Ocean Drilling Program, NASA, and NSF. His association with the Colorado School of Mines and University of North Carolina at Chapel Hill as adjunct professor resulted in the mentoring of thirteen masters and doctoral students. Marty's research interests have evolved during his career. His early work was on the biogeochemistry of sulfur in modern marine sediments.

After joining the USGS, he applied these perspectives on sulfur geochemistry toward understanding the origin of sediment-hosted ore deposits. This interest in ore genesis led to a focus on large scale crustal fluid flow processes that drive not only genesis of some



Martin Goldhaber

ore types, but also impact the modern environment by enriching shallow crustal rocks with potentially toxic constituents. His research then evolved into understanding the environmental impacts of these crustal flow processes. One example of these impacts is the regional enrichment of aquifer rocks in the mid-continent of the U.S. with trace amounts of potentially toxic metals such as Pb and As which can leach into groundwater aquifers. Another example is the enrichment in coal and coal-bearing rocks of the Appalachian Basin in As, Hg, Se, and Tl by fluids mobilized during the Alleghanian orogenic event.

He has researched the mobilization of these coal-related constituents into streams by natural weathering and mining and into the atmosphere and soils by coal combustion. He is currently co-chief of a USGS project to map the inorganic and selected organic constituents in soils of the U.S., and together with the Canadian and Mexican Geological Surveys, all of North America.

Andreas Lüttge's research focuses on the processes that govern fluid/mineral or fluid/rock interactions from low-temperature conditions to the pressures and temperatures of the deep crust. He is particularly interested in the participation of microorganisms in these processes. His work includes various experimental and modeling techniques that he applies to questions of mineral reactions in sedimentary basins, weathering, the fate of nanoparticles in the environment, atmospheric and global change,



Andreas Lüttge

environmental pollution, hydrothermal systems, and the containment of radioactive wastes. Lüttge received his PhD. in 1990 at the University of Tübingen (Germany), spent 3 years as a Humboldt fellow and associate research scientist at Yale University, and currently holds a double appointment as associate professor of Earth Science and Chemistry at Rice University.

Mark McCaffrey received his B. A. degree (1985) from Harvard University, magna cum laude with highest honors in geological sciences, and his Ph.D. (1990) in geochemistry from the Massachusetts Institute of Technology/ Woods Hole Oceanographic Institution Joint Program. Prior to co-founding *OilTracers*, Mark spent 10 years at Chevron and Arco solving a variety of oil exploration and production problems. Mark is a California Registered Geologist (License #5903), a Texas Professional Geoscientist (License #350), and an AAPG Certified Petroleum Geologist (Certificate #5339). He is a senior or co-author of 30 articles on petroleum exploration, reservoir management, oil biodegradation, hazardous waste remediation, paleoenvironmental reconstruction, and marine chemistry. Mark was the 1995 recipient of the Pieter Schenck Award from the European Association of Organic Geochemists for "outstanding work on biomarkers in relation to paleoenvironmental studies and petroleum exploration." In 1998, with project team members, Mark received the Arco Award of Excellence "for developing a new charge and migration model for the Brookian petroleum system, allowing improved charge risk assessment for prospects on the Central North Slope of Alaska. Mark was a 2001-2002 Distinguished Lecturer for the Society of Petroleum Engineers, and was the Chairman of the 2002 Organic Geochemistry Gordon Conference.



Yaoling Niu is a Professor of Earth Sciences at Durham University, UK. He obtained a BSc degree in Geology in 1982 (Lanzhou University, China), an MS degree in Economic Geology in 1988 (University of Alabama, USA), and a PhD degree in Marine Geology and Geophysics in 1992 (University of Hawaii, USA). After one-year postdoctoral research at Columbia University in New York, Yaoling joined The University of Queensland, Australia in 1993 as a Lecturer, and was promoted to Senior Lecturer with tenure in 1997. In 2001, Yaoling joined Cardiff University as a Senior Research Fellow of Natural Environmental Research Council of the UK. In 2003, he gave up this Fellowship and joined University of Houston as an Associate Professor. He then joined the faculty of Durham University in December 2004. Yaoling has lectured on a number of courses including Mineralogy, Petrology, Geochemistry, Global Tectonics and Chemical Geodynamics at both undergraduate and graduate levels in Geology/Earth Sciences Departments in China, USA, Australia and UK since 1982, while studying and conducting research in the intervening years. Yaoling's research uses petrology and geochemistry as a means to understanding how the Earth works on all scales today and in Earth's history. He has published over 60 refereed papers in leading Earth Science journals. He has been honored with guest professorships by several Chinese Universities (China University of Geosciences in Beijing, Northwest University in Xi'an, Nanjing University and Peking University), and honored as an *Outstanding Overseas Chinese Scientist* by Chinese National Science Foundation. He has recently taken the leadership as the Chairman of the IUGS Commission on Solid Earth Composition and Evolution (SECE). Dr. Niu also serves as an Executive Editor of the Chinese Science Bulletin, and is on the Editorial Board of Earth Science Frontiers and the Geological Journal of China Universities. (<http://www.dur.ac.uk/yaoling.niu/index.htm>)



The Environmental Molecular Science Institute At University of Notre Dame

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INTRODUCTION

When most people think of Notre Dame, they picture the soaring spires, flying buttresses, and eerie gargoyles of the medieval cathedral in the center of Paris; or they remember Coach Knute Rockne and one of the most famous and successful college football teams of all time. To others, the name Notre Dame brings to mind a university in the



American midwest that has evolved from humble beginnings as a men's undergraduate school located in a frontier trading-post town to become an international center of learning and world-class research. The University of Notre Dame, which was founded in 1842 by Edward Sorin, a French priest of the Congregation of Holy Cross, is an independent Catholic university located in northern Indiana, approximately 90 miles east of Chicago. Notre Dame has an outstanding undergraduate and graduate student population. Sixty-nine percent of incoming freshmen are in the top 5 percent of their high school graduating classes, and Notre Dame is one of a handful of truly international universities, with a student body drawn from all 50 states and 100 countries. Notre Dame ranks in the top 20 among all American colleges and universities in size of endowment and in annual voluntary support.

The focus of geochemistry research at Notre Dame is the Environmental Molecular Science Institute (EMSI; www.nd.edu/~emsi), funded by the U.S. National Science Foundation and the U.S. Department of Energy with additional support from the University of Notre Dame. The NSF/DOE Environmental Molecular Science Institutes Program currently funds seven institutes across the United States, bases at Princeton University, The Ohio State University, The New York at Stony Brook University, University of California State University, and EMSIs include partnerships with academia, national laboratories, and the general public. The goal of each Institute is to increase our molecular-level understanding of anthropogenic processes in the environment. A molecular-level understanding of environmental processes to prevent and remediate problems caused by so-

The scientific mission of the University of Notre Dame is to determine the effects of nano- and micro-particles (e.g., bacteria, natural organic matter, and mineral aggregates) on radionuclide transport in the environment. The Institute blends the science and engineering expertise present at Notre Dame with those of Argonne and Sandia National Laboratories, as well as at DuPont and other national laboratories. The Institute integrates traditional macroscopic and microscopic techniques with state-of-the-art molecular-scale approaches such as x-ray absorption spectroscopy, atomic force microscopy, and molecular dynamics modeling. Both undergraduate and graduate students take part in Institute-related research. Students in the Institute experience an integrated interdisciplinary research environment, as the Institute brings together scientists and engineers with expertise in a wide variety of environmental disciplines, including aqueous and organic geochemistry, mineralogy, geomicrobiology, microbiology, physics, actinide chemistry, surface chemistry, hydrology, environmental engineering, biochemistry, and molecular dynamics modeling. Graduate students are encouraged to participate in a research internship program, which enables graduate students to conduct research with our national laboratory and industry partners. The Institute maintains an extremely well-equipped, centralized analytical facility at Notre Dame (Figure 1), providing researchers with powerful approaches for studying molecular-scale environmental geochemistry. Students also work in Notre Dame's Center for Environmental Science and Technology (CEST; www.nd.edu/~cest), which provides additional analytical instruments in a well maintained environment that is 'free of charge' except for consumables. The EMSI is also the focus for a range of innovative educational and outreach programs, and this report will describe these activities as well.

Figure 1 (opposite). *The Environmental Molecular Science Institute laboratory at University of Notre Dame. Clockwise from top left: a Research Experience for Undergraduates (REU) student using the EMSI environmental SEM to study biofilm morphologies; a high school outreach program participant conducting wet chemistry experiments; a wide-angle view of the EMSI lab with a range of tools for microbiological and geochemical procedures; EMSI postdoc Dr. Ben Turner analyzing dissolved metal concentrations using the EMSI inductively-coupled plasma optical emission spectrometer; an EMSI research technician obtaining spectra using a UV-vis spectrophotometer.*

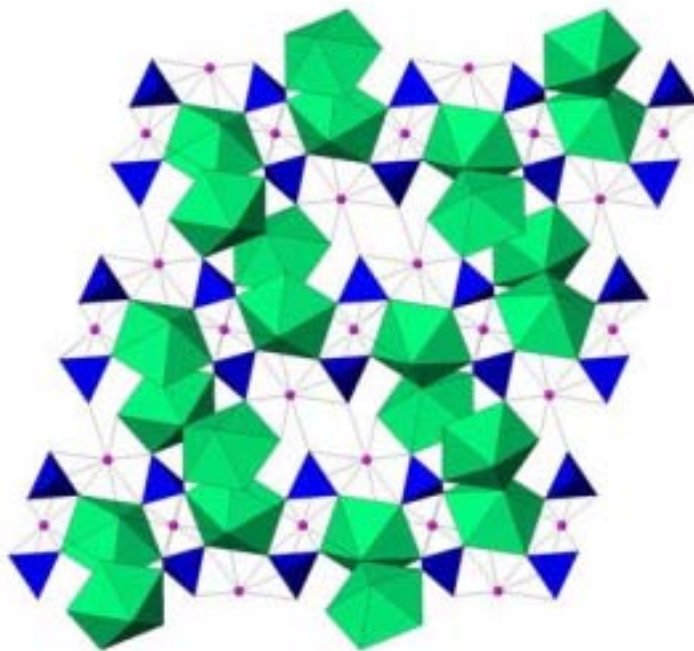


Figure 2. *Framework of neptunyl and sulfate polyhedra in the structure of $\text{Na}_2(\text{NpO}_2)_2(\text{SO}_4)_2(\text{H}_2\text{O})$ (Forbes et al. 2006).*

INTELLECTUAL FOCUS AND GOALS

Liquid and solid wastes from industry and nuclear activities have severely contaminated a number of groundwater systems with heavy metals and actinides. The inability to accurately predict the fate of these elements in the subsurface can lead to ineffective remediation efforts, and has been a major concern in planning a high level nuclear waste repository. Generally, geochemical transport models consider only two possible chemical fates for a contaminant: either mobile as a dissolved species, or immobile due to adsorption or precipitation onto the solid geologic matrix. However, subsurface environments also contain nano- and micro-particles that are composed of mineral, organic, and microbiological phases. These particles can be mobile in the subsurface, and they can markedly affect metal transport. Development of accurate predictive models of the effects of these particles requires a quantitative, molecular-level understanding of the diverse (bio)geochemical interactions between metals (including the actinides) and small particles. Institute research focuses primarily on the actinides uranium (U) and neptunium (Np), and on the metals cadmium (Cd), copper (Cu), and lead (Pb). We have identified these elements for the primary focus of Institute research in part because of their importance as environmental contaminants (or potential contaminants), but also because of their diverse and complex chemical behaviors. In the cases of U and Np, oxidation state controls their geochemical behavior; reduced (IV) forms of these elements are essentially insoluble, whereas the oxidized forms (V, VI) can be much more mobile.

The scientific activities of the Institute can be classified under two broad umbrellas: 1) Inorganic system studies in which Institute researchers investigate the homogeneous nucleation and stability of radionuclide-bearing nano- to micro-scale aggregates; and 2) mixed organic/microbiological systems in which researchers investigate the effects of natural organic matter (NOM) and bacteria, in the presence and absence of nano- to clay-sized mineral particles, on processes such as the heterogeneous nucleation, stability, and structure of contaminant-bearing particles, the sorption of the contaminants to NOM and bacteria, redox effects driven by NOM and bacteria, and column flow experiments in which our understanding of nano- and micro-particle effects on contaminant transport can be tested. We describe some of the research results from these investigations, however this article necessarily focuses on that fraction of the research that has already been published, with brief references to ongoing work.

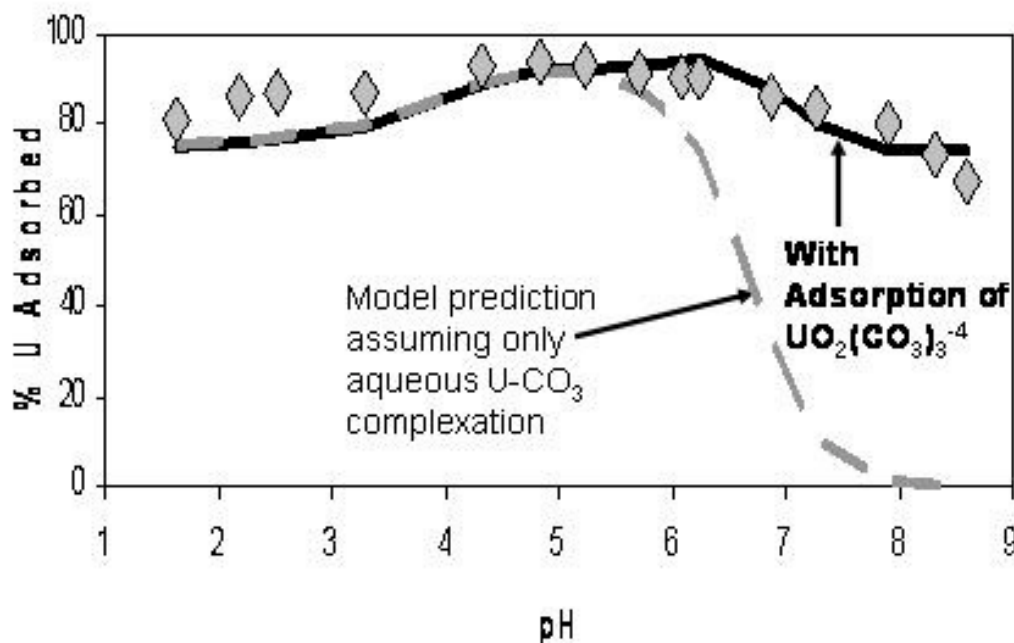


Figure 3. Measured adsorption of aqueous U(VI) onto *Bacillus subtilis* bacterial cells (0.5 gm wet mass/L) suspended in solutions in equilibrium with atmospheric CO₂. Dashed curve represents a thermodynamic model prediction for the extent of adsorption assuming that uranyl-carbonate complexes do not adsorb and remain in solution; Solid curve represents the best-fitting model constructed assuming that uranyl-carbonate bacterial surface complexes form. Data suggest that significant adsorption of aqueous uranyl-carbonate complexes onto the bacterial cell wall can control U speciation and mobility in near-neutral waters. From Gorman-Lewis et al. (2005b).

Each of the projects that are described below represents collaborative interdisciplinary research between at least two Institute members, and more typically the projects bridge the expertise of three or four researchers located at Notre Dame, Argonne, Sandia, and/or DuPont. Environmental molecular science research is inherently interdisciplinary due to the complexities and heterogeneities inherent in natural environments. Research projects sponsored by EMSI address these complexities through the unique perspectives offered by collaborative investigations.

SCIENTIFIC ACTIVITIES

1. Inorganic System Experiments

The assumption that metal ions are transported through the envi-

ronment largely as dissolved ions in idealized solutions has long been known to be only partially correct. Small aggregates and colloids also often play an important role in environmental processes and are common particularly for trivalent and tetravalent species (Lieser and Hill, 1992; Neck and Kim, 2001). Aggregation effectively concentrates the metal-ion on a local scale, thereby providing a pathway for precipitation and immobilization. Aggregates of metal ions in geological solution are probably the precursors of homogeneous mineral precipitation.

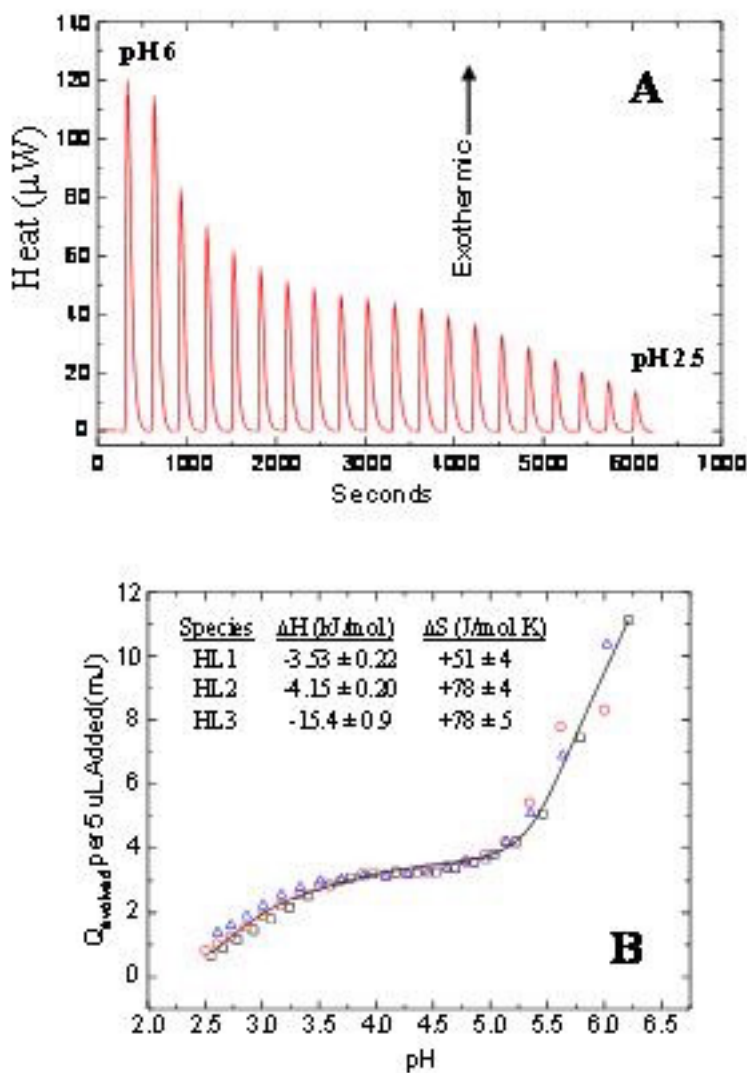


Figure 4. A) Raw data from a typical low pH proton adsorption calorimetric titration experiment, showing heat associated with adsorption of protons onto functional groups on the bacterial cell wall of *Bacillus subtilis*. Data show continuous uptake of protons, and that the cell wall functional groups are not fully protonated even under the lowest pH conditions of these experiments. B) Corrected heat evolved from three low pH proton adsorption calorimetric titration experiments involving *B. subtilis*, with the curve representing the best fit to the data assuming three types of protonation sites each with their own discrete pKa value. Each figure indicates that protonation reactions are exothermic, with heats comparable to those associated with protonation of multifunctional organic acids. The calculated site-specific enthalpies and entropies of protonation are listed in (B), and the low values for S suggest hydrogen bonding between functional group sites. From Gorman-Lewis et al. (2005c).

It is likely that aggregates of metal ions with dimensions in the 10s of Å are of fundamental importance for understanding of the mobility of U, Np and Pb in many geologic fluids, as well as the homogeneous nucleation of low-temperature minerals. Under specific conditions, such aggregates may persist in solution and dominate the transport of the metal ions. Little is known about the formation, structure, and thermodynamic stability of suspended metal-containing aggregates in solution, although their ultimate fate rests primarily on just such factors.

Institute members are examining aggregates of metal ions in solutions to determine their composition, atomic structure, formation and stabilization mechanisms, and long term fate in solution. This is a difficult undertaking because few techniques present the possibility of detecting and characterizing aggregates containing tens to hundreds of atoms in solution. Various synchrotron-based spectroscopic techniques provide information concerning the oxidation state of a metal ion in solution, as well as the coordination sphere within 3-5 Å of the metal ion, but fail to provide the longer-range information necessary to characterize the size, shape and composition of the aggregate. Solid state structures can provide useful models for metal ion coordination and aggregation in solution.

Perhaps the most effective approach to understanding the structures and chemistry of metal ion aggregates formed in solution is to combine conventional X-ray diffraction studies with synchrotron-based X-ray scattering experiments. This requires crystallization of metal ion aggregates from solution into extended three-dimensional molecular crystals. Provided that it is possible to coax the aggregates from solution into a crystal, single-crystal X-ray diffraction then can provide the details of the atomic-scale structure and chemical composition of the aggregate. Then, knowing the size and shape of the aggregate of metal ions based upon the derived structure, a synchrotron technique such as small angle X-ray scattering (SAXS) will demonstrate the presence of the aggregate in solution, and will provide the pos-

Figure 5. A molecular simulation schematic of a peptidoglycan chain attached to a teichoic acid dimer. Peptidoglycan and teichoic acid are the major metal binding constituents of the *B. subtilis* cell wall. This figure depicts four peptidoglycan dimers that are linked/bridged together to form more of a "fabric" representation of the cell wall, with an example of how a Cd^{+2} ion (green sphere) would interact with the functional groups present. From Johnson et al. (2005).

sibility of tracking the aggregate through geochemical reactions.

An example of the combination of single-crystal X-ray diffraction and SAXS to document metal ion aggregation in solution has recently been published by members of the Institute (Burns et al. 2005; cover of this *GN* issue). In this study, solutions containing uranyl or neptunyl ions in alkaline conditions were treated with peroxide, which created unprecedented nanospherical particles containing 24, 28 or 32 metal ions, as well as more than 150 atoms of oxygen. The syntheses were done under ambient conditions, and the compositions of the reactants are broadly consistent with high-level nuclear waste that currently resides in below-ground storage tanks at Hanford and elsewhere. The intense radioactivity of the waste can create significant peroxide in water through alpha-radiolysis. The nanospheres crystallized and it was possible to determine the atomic-scale structure of the clusters using X-ray diffraction data collected using a CCD-based detector. SAXS studies of solutions clearly indicated the presence of geometrically identical clusters in solution, providing strong evidence that the clusters self-assembled in solution, and eventually found their way into extended crystals. Discovery of these nanostructures, and the elucidation of their structures and chemical compositions, provides a unique opportunity to study the behavior of well characterized aggregates in solution, specifically their fate under changing solution conditions, their sorption onto mineral surfaces, and their reaction with minerals with a wide range of chemical compositions. Ongoing research by Institute members is addressing the potential for transport of uranyl peroxide nanospheres in environmental systems.

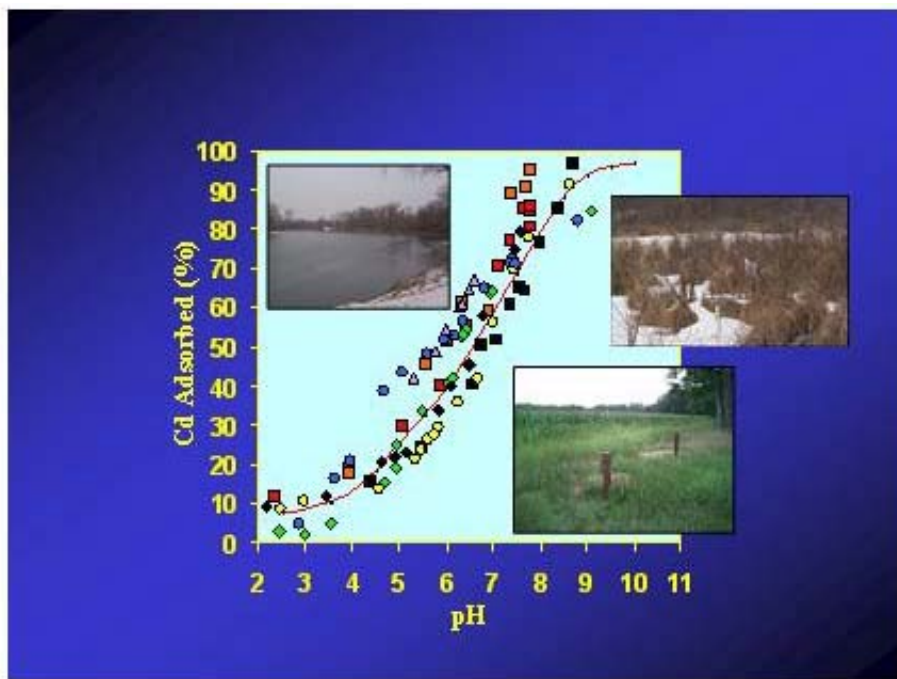
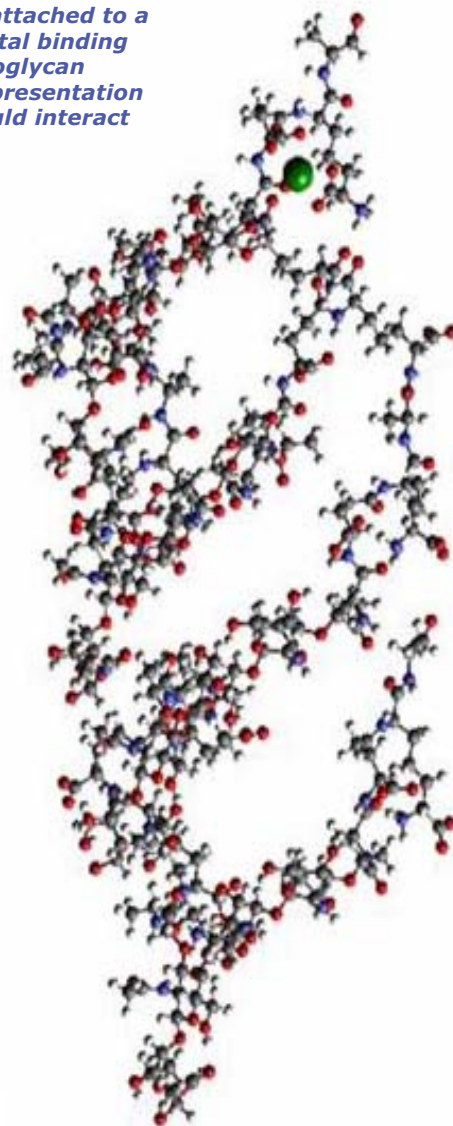
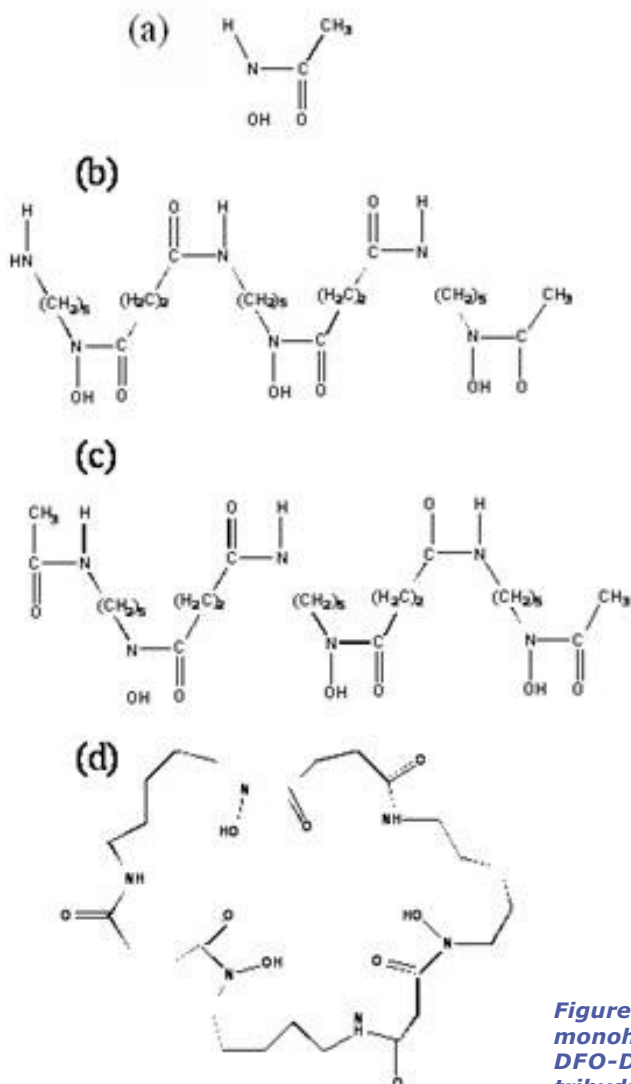


Figure 6. Cd adsorption onto bacterial consortia cultured from soil and aquatic environments, three of which are depicted above. All Cd adsorption experiments were conducted using 10 ppm Cd and 10 g/L consortia (wet mass) in a suspension of 0.1 M $NaClO_4$. The consortia were grown using soil broth (SB) or trypticase soy broth (TSB) with 0.5% yeast extract. ■ = Forest Soil #1, SB, ■ = Wastewater Effluent, TSB, purple triangle = Wastewater Effluent, SB, green diamonds = Forest Soil #2, SB, ● = River Water, SB, ● = Wetland Water, TSB, black diamond = Wetland Soil, SB, ■ = Wetland Water, SB. The solid line represents the best-fitting adsorption edge that is calculated using 'universal' functional group site concentrations and binding constants. After Borrok et al. (2004).

In the case of neptunium, the pentavalent cation is highly soluble and stable in groundwater, and is of considerable concern for the long-term storage of nuclear waste because its half-life is greater than 2 million years. There are about 200 uranyl minerals known (minerals that contain hexavalent uranium), and the structures have been reported and refined for close to half of the known species (Burns, 2005). It is possible to use these structures to gain considerable insight into the coordination chemistry of hexavalent uranium in solution. Neptunium, however, is not a natural element, and there is no database of mineral structures to guide understanding of its behavior in natural systems. It is tempting to assume uranyl minerals are an analogue for neptunium in natural systems, but Institute research is showing that such an assumption would be unwise, because the coordination chemistry of pentavalent neptunium is likely significantly distinct from hexavalent uranium. It is clear that a significantly enhanced understanding of the crystal chemistry of neptunium will serve as a cornerstone for understanding neptunium complexation in solution.

Institute researchers are examining the crystal chemistry of pentavalent neptunium in crystals with environmentally relevant chemical compositions – specifically oxyhydrates, phosphates, and sulfates. Crystals are first synthesized using mild hydrothermal techniques in special laboratories designed for the safe handling of radioactive materials. When suitable crystals are obtained, X-ray diffraction data is used to elucidate the entire crystal structure, and to determine bond lengths with estimated errors of a few hundredths of an angstrom. Findings to date are clearly demonstrating that the coordination environments about pentavalent neptunium depart significantly from those of hexavalent uranium (Forbes and Burns, 2005; Forbes et al. 2006). Both contain the well-known actinyl ion in which the cation is strongly bonded to two atoms of oxygen, forming approximately linear ions. However, the bonds within the neptunyl ion are a little weaker than those in the uranyl ion, and this results in so-called cation-cation interactions, in which one neptunyl ion actually coordinates another. Such a coordination geometry is unknown in uranyl minerals, and occurs in only a couple of percent of synthetic uranyl phases. However, approximately fifty percent of pentavalent neptunium structures have cation-cation interactions.



Such a coordination geometry is unknown in uranyl minerals, and occurs in only a couple of percent of synthetic uranyl phases. However, approximately fifty percent of pentavalent neptunium structures have cation-cation interactions.

A recent study by Institute members (Forbes et al., 2006) has revealed the structures of novel neptunyl sulfates that contain sulfate and neptunyl polyhedra that are linked into infinite three-dimensional frameworks (Figure 2). Cation-cation interactions dominate the linkages between the neptunyl polyhedra, and this new structure type shows unusual magnetic ordering which may be linked to the cation-cation interactions.

2. Organic/Microbiological System Experiments

Natural organic matter (NOM), bacteria, and clay-sized mineral particles represent nano- to micro-scale colloids that are ubiquitous in groundwater environments and can have a significant impact on the speciation and mobility of metal and radionuclide contaminants. A number of research projects at the EMSI aim to understand the effects of these particles on the speciation and transport of actinides (U and Np), heavy metals (Cd, Cu, Hg, and Pb), and metal nutrients such as Fe.

i) Studies of molecular-scale mechanisms of bacterial surface adsorption

Figure 7. Molecular structure of (a) aHA (siderophore-like monohydroxamate), (b) DFO-B (linear trihydroxamate), (c) DFO-D₁ (linear trihydroxamate), and (d) DFO-E (cyclic trihydroxamate).

Bacteria are present in a wide range of low-temperature geologic systems, and adsorption of aqueous metal cations onto bacterial cell walls can influence the speciation and mobility of metals in the environment. Although the potential influence of bacteria on geochemical processes has been realized for decades, quantitative models of the effects of bacterial adsorption on metal distributions in water-rock systems still do not exist. EMSI research has focused on two major obstacles which must be overcome in order to include bacterial adsorption effects in geochemical models of mass transport: 1) characterization of the molecular-scale mechanisms of proton and metal cation adsorption onto bacterial cell walls so that accurate adsorption reactions can be formulated and so that stability constants for the important metal-bacterial surface complexes can be determined; and 2) determination of the existence of commonalities between the adsorption behavior of different bacterial species. Although some constraints have been placed on bacterial adsorption mechanisms, the complexity of the cell wall and its associated structures make the task especially challenging. Because we know so little about adsorption mechanisms even for the relatively few species of bacteria that have been studied, it is not yet clear if adsorption mechanisms differ from species to species. The number of bacterial species of environmental and geologic interest is huge and undetermined, and if each species exhibits unique adsorption behavior, then it would be a nearly impossible task to develop quantitative models of bacterial adsorption in realistic systems.

Bulk Adsorption Measurements

The EMSI has sponsored a range of research projects that involve the measurements of proton and metal adsorption onto bacterial surfaces. These data provide constraints on the thermodynamic properties and surface concentrations of bacterial surface complexes, and these experiments can also provide constraints on adsorption reaction stoichiometries. For example, Fein et al. (2005) conducted potentiometric titrations using the Gram-positive aerobic species *Bacillus subtilis*, covering the pH range 2.1 to 9.8, at ionic strengths between 0.01 and 0.3 M. This study documented significant adsorption of protons over the entire pH range, including to the lowest pH values examined, indicating that proton saturation of the cell wall does not occur under any of the conditions of the experiments. Electrophoretic mobility measurements indicated that the cell wall is negatively charged, even under the lowest pH conditions studied.

Fein et al. (2005) modelled the potentiometric titration data using three significantly different approaches: a Non-Electrostatic Model, a Constant Capacitance Model, and a Langmuir-Freundlich Model. The approaches differ in the manner in which they treat the surface electric field effects, and in whether they treat the proton-active sites as discrete functional groups or as continuous distributions of related sites. Each type of model tested, however, provides an excellent fit to the experimental data, indicating that titration data alone are insuffi-

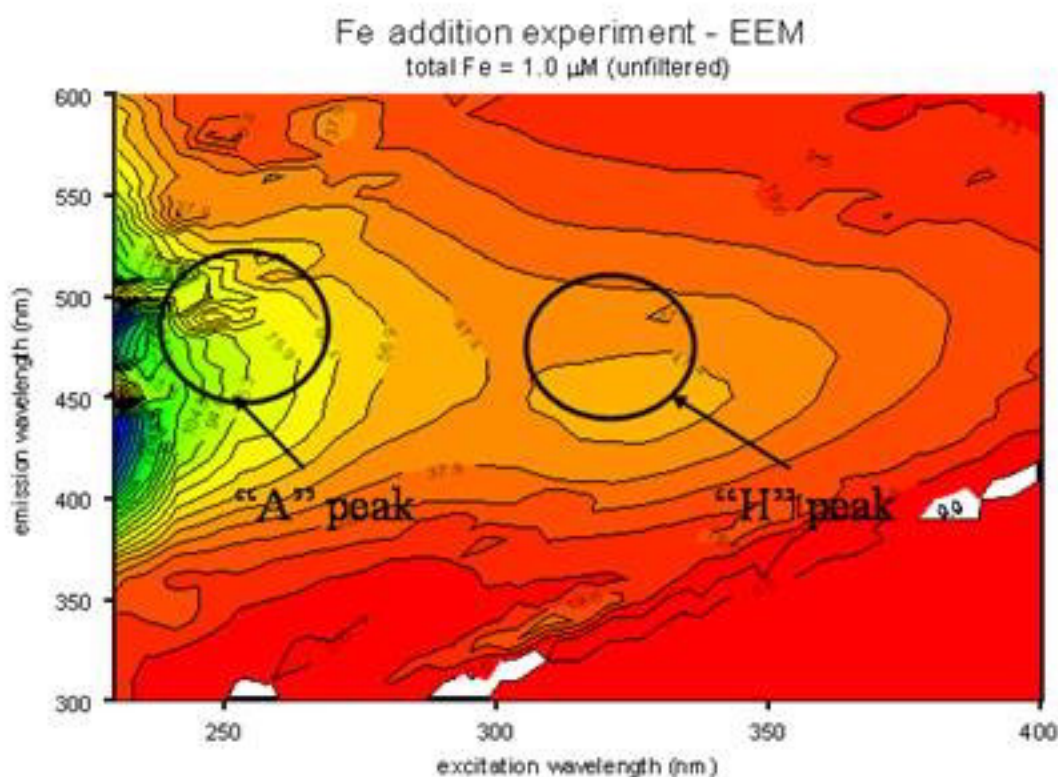


Figure 8. A typical 3-D fluorescence EEM plot of a humic/fulvic NOM sample. The x-axis is the excitation wavelength, the y-axis the emission wavelength, and the z-axis is the fluorescence intensity in quinine sulfate units. The two peaks occur at excitation/emission pairs of 320/450 nm (labeled "H" peak) and 230/435 nm (labeled "A" peak).

cient for characterizing the molecular-scale reactions that occur on the bacterial surface. Spectroscopic data on the molecular-scale properties of the bacterial surface are required in order to differentiate between the underlying mechanisms of proton adsorption inherent in these models.

The EMSI has also sponsored investigations of U and Np adsorption onto bacterial surfaces to determine the effects of bacterial adsorption on the mobility and environmental speciation of these radionuclides. Np and U exhibit markedly different adsorption behaviors onto the Gram-positive species *B. subtilis*. Np adsorbs relatively weakly, with adsorption that is strongly dependent on ionic strength (Gorman-Lewis et al., 2005a). Np uptake is primarily the result of adsorption, however Np uptake onto the cells under low pH high ionic strength conditions is consistent with bacterially influenced reduction of the Np (V) to Np (IV). U, in contrast to Np, adsorbs strongly to the bacterial surface over a wide pH range, as depicted in Figure 3 (Gorman-Lewis et al., 2005b). These are rather surprising results because in oxygenated, CO₂-rich systems, negatively charged uranyl-carbonate complexes dominate the aqueous uranium speciation, and it is commonly assumed that these complexes exhibit negligible adsorption onto negatively charged surfaces such as bacteria. Thermodynamic modeling of the U adsorption data suggests that uranyl-hydroxide, uranyl-carbonate and calcium-uranyl-carbonate species each can form stable surface complexes on the bacterial cell wall, and their presence may dramatically alter predictions of uranium mobility in near-surface environments.

X-ray Absorption Spectroscopy

Although bulk adsorption experiments represent a powerful approach for quantifying stability constants of metal adsorption reactions, the data provide relatively weak circumstantial constraints on the molecular-scale mechanisms responsible for the metal adsorption. More rigorous constraints on adsorption mechanisms are offered by a range of complementary experimental approaches, and a number of these approaches have been applied successfully to examine metal-bacterial adsorption reactions. X-ray absorption spectroscopy (XAS) has been used to constrain the binding environment for metal cations on cell wall functional groups (e.g., Sarret et al., 1998; Hennig et al., 2001; Kelly et al., 2002; Panak et al., 2002a; 2002b; Boyanov et al., 2003; Templeton et al., 2003; Francis et al., 2004). Spectroscopic data provide more direct evidence of the metal coordination environment than do bulk adsorption measurements. However, due to the complexity of the cell wall binding environments, and due to the fact that XAS yields an averaged binding environment, the experimental results from XAS can be complex and difficult to interpret. For example, although XAS has been used successfully to demonstrate the importance of carboxyl and phosphoryl binding sites for U and Cd on the bacterial cell wall of *Bacillus subtilis*, significant uncertainties exist regarding the metal:ligand stoichiometry involved in binding (Kelly et al., 2002; Boyanov et al., 2003). The XAS data require at least three distinct binding sites over the pH range of 3.5 to 7.0, and the data do not point to the type of binding complexity that might be expected for a cell wall which contains functional groups that deprotonate continuously over a wide pH range. The EMSI is sponsoring current research projects that investigate the binding mechanisms responsible for Np, U, and Cd uptake by cell walls of a range of bacterial species, both Gram-positive and Gram-negative, as well as by bacterial consortia from natural environments.

Calorimetry Studies

Calorimetric measurements of bacterial surface protonation reactions offer another relatively untapped resource for constraining proton adsorption mechanisms. Calorimetry measurements of proton adsorption onto bacterial cell walls not only can provide rigorous constraints on the extent of bulk proton adsorption, but interpretation of these data using a surface complexation modeling approach can yield site-specific enthalpies and entropies of proton adsorption onto the bacterial surface functional groups. These data can be interpreted to yield information on proton coordination environment, as well as the temperature dependence of the protonation reactions. In Institute-sponsored research, Gorman-Lewis et al. (2005) have conducted the only calorimetric study of site-specific bacterial surface protonation to date. Their results (Figure 4) indicate that the protonation reaction is exothermic, with calculated site-specific entropies of protonation that are relatively small. This suggests that the functional groups on the bacterial surface behave more like multifunctional organic acids with nearby proton-active sites rather than simple monofunctional acids with a single isolated functional group. Hydrogen bonding between protonated and deprotonated sites likely occurs as reflected by the relatively small entropies of protonation. The calorimetry results suggest that the use of multifunctional organic acids likely represent better analogues than monofunctional acids in modeling the acidity behavior of the functional groups present on bacterial surfaces.

Molecular Modeling Approaches

A significant and complementary component of EMSI research on metal-bacterial adsorption reactions involves molecular simulation methods, which can provide a more detailed and atomistic understanding of how metal cations interact with specific functional group types within the bacterial cell wall. Molecular modeling methods can be used to calculate the total potential energy of a molecular cluster or of a periodic system through either molecular mechanics or quantum mechanics. Molecular mechanics evaluates the interactions of individual atoms or mol-

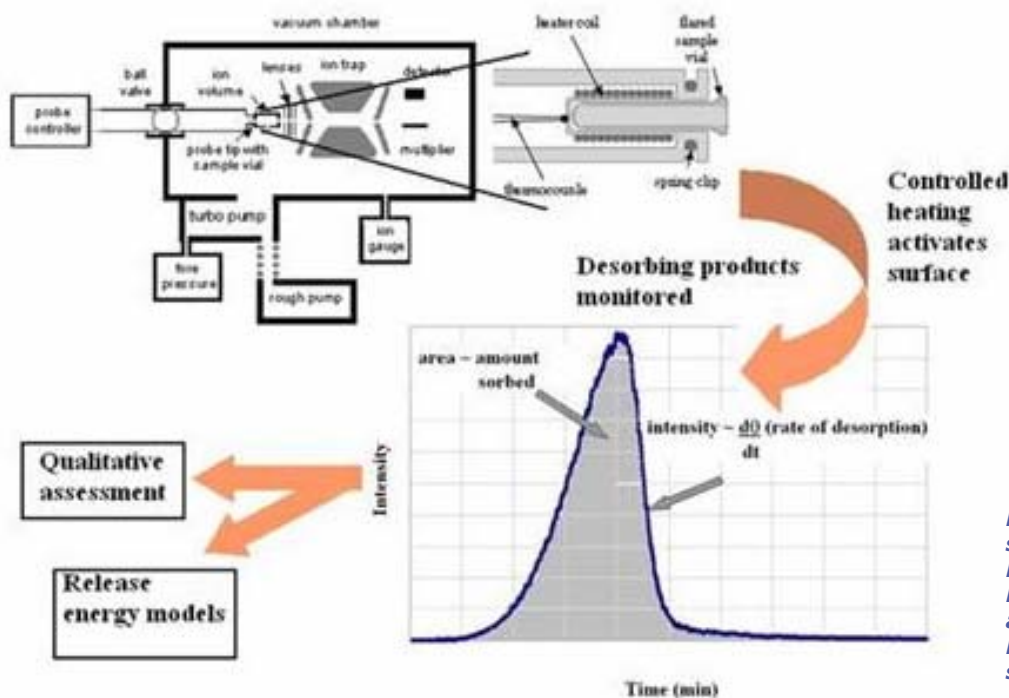


Figure 9. Schematic representation of the Thermal Programmed Desorption – Mass Spectrometer analysis approach for characterizing Hg sorption onto sediment surfaces.

ecules while quantum methods extend the simulation tools to the electron level, evaluating the electronic structure of the system (e.g., Cygan, 2001). Through molecular mechanics methods, such techniques as energy minimization, conformational analysis, and molecular dynamics can be applied to a system of interest, for example those involving many hundreds and thousands of atoms of macromolecules representing a bacterial surface. EMSI research includes investigations of the atomic-scale interactions that occur between cations and the metal-binding cell wall components common to many gram-positive bacteria. The adsorption of Cd^{2+} and Pb^{2+} onto peptidoglycan and teichoic acid components of the bacterial cell wall were examined using classical energy force-field methods in order to determine relative binding energies and structural configurations of the cell-wall components, both with and without the metals present (Johnson et al., 2005). The application of force field methods allows us to examine large and complex behavior of macromolecules such as the linked peptidoglycan dimers in Figure 5. These methods are useful for studying the adsorption of a cation when multiple ligands are available, the rigidity of the major cell wall constituents, and adsorption strength, binding distance and coordination on the atomic level without the computational cost and limited system size required for quantum methods based simulations of the same system. Future research includes the improvement of force field parameters, larger system sizes, multiple metal sorption, and competitive sorption processes.

Scaling Issues: Column Studies

The scientific objective of the EMSI is to improve our understanding of the molecular-scale mechanisms that control heavy metal and radionuclide transport in the subsurface. Most of the EMSI research projects attempt to isolate these mechanisms in experiments, however we also are using experiments involving columns filled with geologic media to test our ability to apply our new-found molecular-scale understandings to account for particle and contaminant transport on a macroscopic scale (Turner et al., 2005a; 2005b). For example, we have used this approach to determine whether equilibrium thermodynamics and our calculated metal-bacterial thermodynamic parameters can be used to accurately account for metal and bacterial transport through columns that contain either quartz grains or ferrihydrite-coated quartz grains. Model simulations that are calculated assuming attainment of adsorption reaction equilibrium and using stability constants and site concentrations derived from our previous research predict metal breakthrough behavior in good agreement with experimental results. Since flow rates in the column experiments were fast compared to most flow rates in geologic aquifers, these experiments suggest that the kinetics of metal redistribution are fast enough that the assumption of thermodynamic equilibrium is appropriate for modeling coupled solute-colloid transport in most aquifers.

ii) The search for bacterial adsorption commonalities

Most experimental studies of metal adsorption onto bacterial cell walls involve only a single bacterial species. One of the most problematic obstacles to the application of surface complexation modeling to realistic systems is that a given bacteria-bearing natural system can contain a large number of different bacterial species, and the number of species of environmental interest is huge and undetermined. If bacterial surfaces are unique and if each species exhibits unique adsorption properties, then it would be a Herculean task to determine the binding site concentrations and proton and metal binding constants for each bacterial species of environmental interest. Experimentation on dozens of different bacterial species would be necessary just to describe the metal adsorption behavior in a single environment. If bacterial species differ significantly from each other in their adsorptive behaviors as do mineral surfaces, then the complexities of realistic systems would make it virtually impossible to model metal speciation and distribution on a molecular-scale due to practical computational limitations. Conversely, application of too simple a model that does not account for surface and solute speciation changes with changing subsurface conditions can lead to inaccurate predictions of metal speciation and mobility (e.g., Bethke and Brady, 2000; Koretsky, 2000).

A component of EMSI research is aimed at finding commonalities in adsorption behavior between bacterial species such as that proposed by Yee and Fein (2001) who hypothesized that a common mechanism of adsorption exists for a wide range of bacterial species. EMSI sponsored the research conducted by Borrok et al. (2004), who measured H⁺ and Cd adsorption onto bacterial consortia from a range of natural environments. Their results indicate that the consortia adsorb similar extents of protons and Cd, and that the adsorption onto all of the consortia can be modeled using a single set of stability constants (Figure 6). In addition, Borrok et al. (2005) compiled all currently available potentiometric titration datasets for individual bacterial species, bacterial consortia, and bacterial cell wall components. Borrok et al. (2005) found that the total concentrations of proton-active functional group sites for the 36 bacterial species and consortia tested are remarkably similar, and they derive an averaged internally-consistent set of 'universal' thermodynamic proton binding and site density parameters for modeling bacterial adsorption reactions in geologic systems. Current EMSI projects on adsorption commonalities involve using x-ray absorption spectroscopy to identify binding environments of heavy metals on gram-negative bacterial species as well as on mixed consortia of bacteria grown from natural settings. The objective of this work is to determine if the similar adsorption behavior that was observed by Yee and Fein (2001) and by Borrok et al. (2004) is caused by universal adsorption mechanisms.

iii) Effects of bacterial siderophores on trace metal and radionuclide mobility in the subsurface.

Siderophores (Greek for iron-carriers, see Figure 7) are low molecular weight organic ligands that are produced by microorganisms and some plants under iron-limited conditions, and that are commonly present in soil systems. Siderophores have a high specificity for Fe(III), relative to Fe(II); siderophore Fe(III) 1:1 complex stability constants range from 10²³ to 10⁵². Siderophores also can form stable complexes with other metals, such as Al(III), Ga(III) and In(III), Cd(II), and Pb(II). This ability to form stable metal-ligand complexes suggests that siderophores may influence metal mobility in soils by affecting rates of mineral weathering, and/or by either enhancing or inhibiting metal adsorption to environmental particles. Ams et al. (2002) showed that when an aerobic *Pseudomonas mendocina* bacterium is highly Fe stressed, meaning that little Fe is available, the individual bacterial cells tend to produce relatively large quantities of siderophore; i.e., high production per cell. When there is ample Fe available, there is less siderophore production per cell, but because the overall population size is greater, there can be more total siderophore produced.

EMSI-sponsored research has investigated the effects of the trihydroxamate siderophore desferrioxamine -B (DFO-B) on the dissolution of the highly insoluble Pb-phosphate mineral, pyromorphite. Phosphate addition as the mineral hydroxyapatite to soils has been suggested as a means to remediate highly Pb-contaminated soils. As the apatite dissolves to release phosphate, highly insoluble and supposedly non-bioavailable particles of pyromorphite form (e.g., Manecki et al, 2000). Our studies have shown that DFO-B, which is known to be produced by fungi in aerobic soils, rapidly dissolves Pb out of pyromorphite, hence mobilizing the Pb and perhaps making it more bioavailable to higher organisms.

EMSI researchers also have been investigating the effects of hydroxamate siderophores on adsorption of Pb and Cd to kaolinite clay (Hepinstall et al., 2005 and work by Maurice/Bunker groups in prep.) Potential co-adsorption of siderophore-metal complexes to the mineral surface could enhance metal adsorption. Alternatively, if siderophores in solution compete with mineral surface adsorption sites, or if metal-siderophore complexes adsorb less strongly than the metals alone, then metal adsorption may be inhibited. Hepinstall et al. (2005) found that that the hydroxamate siderophores appear to have little effect on Cd adsorption to kaolinite. However, effects on Pb adsorption can be pronounced, and vary with pH. Batch adsorption studies indicate that Pb sorption to kaolinite is unaffected by DFO-B at pH values less than 4.5, where there is little Pb complexation by DFO-B in solution, and that sorption is slightly enhanced in the presence of DFO-B around pH 5-6, and decreases at pH ≥6.5 (Hepinstall et al.,

2005). These observations were confirmed by X-ray fluorescence measurements. Current EMSI-sponsored research involves synchrotron based XAS to determine the local binding environment of Pb in solution and at the clay surface, in the presence and absence of DFO-B. XAFS indicates that Pb adsorbs as an inorganic species at pH < 4.5, as several different species at pH 5-6, and primarily as a ternary surface complex with DFO-B at pH \geq 6.5. This confirmation of a ternary surface complex again highlights the importance of a molecular-based approach for understanding metal adsorption and mobility in the subsurface. Current EMSI research expands this research to study Fe and U binding by hydroxamate siderophores, and to quantify the effects of siderophores on metal adsorption to the swelling clay montmorillonite.

iv) Molecular-based studies of interactions between natural organic matter, minerals, bacteria, and metals

The Note Dame EMSI has also focused a good deal of research on understanding the controls on organic- metal-mineral- and/or microbial interactions. Natural organic matter (NOM) is ubiquitous in aquatic and terrestrial environments, and it plays an important role in many biogeochemical processes, affecting the fate and transport of metals, radionuclides, and hydrophobic organic compounds (Cabaniss et al. 2000 and references therein); helping to control the penetration of potentially harmful UV radiation in surface waters (Scully et al., 1995), and serving as a primary C source to microorganisms (Young et al., 2005). The effects of NOM on water treatment processes and the removal of NOM from drinking water have been the topics of much ongoing investigation in environmental engineering. NOM can present problems in drinking water by, for example, clogging filtration systems, serving as a C source to bacteria within distribution systems, and leading to disinfection byproducts when bromide and chloride react with humic substances. Our EMSI-related research has shown, for example, that Fe affects the light absorbance properties, fluorescence, and molecular weight distribution of (NOM) (Anthony et al., 2005). Addition of Fe(III) to 5 and 10 mgC/L humic/fulvic acid at pH 5.5 causes absorbance of visible light to increase, fluorescence intensity of peaks at excitation/emission wavelengths 230/435 ("A" peak) and 320/450 ("H" peak) to decrease (see Figure 9), and a small shift from intermediate to higher MW components. Ongoing research by EMSI researchers is focusing on the effects of Cd, Pb, and a host of inorganic anions on these NOM properties. We have also investigated how photodegradation (Pullin et al., 2004), gamma irradiation, and sonolysis (Kreller et al., 2005) of NOM each affect NOM properties and how photoirradiation affects adsorption of NOM to Fe oxide surfaces (Pullin et al., 2004). Finally, we have investigated the adsorption of NOM to non-metabolizing bacterial surfaces (Maurice et al., 2004), the effects of Cd on this adsorption process (Frost et al., 2004), and the uptake of NOM by natural assemblages of metabolizing bacteria (Young et al., 2004, 2005).

v) Industry Collaboration: Hg adsorption modeling

Mercury contamination of aquatic systems has become a widespread environmental problem. Past industrial uses of mercury compounds, past application of organomercurial pesticides, and the continued combustion of materials with trace levels of mercury have resulted in high concentrations of mercury in aquatic systems. This mercury has biomagnified up the food chain and now poses a threat to human health. Because mercury interactions in aquatic systems are not completely understood, it is difficult to predict both the speciation and the behavior of mercury compounds in the natural environment. Recent research has found that sediments act as both sinks and sources for mercury, thereby, impacting aquatic life for extended periods of time (Ullrich et al., 2001). Given the long term impacts of mercury contaminated sediments, it is clear that further study of the distribution and physical availability of mercury in these sediments is necessary if they are to be successfully remediated and managed.

EMSI-sponsored research aims to relate a molecular-scale understanding of the adsorption reactions of inorganic mercury (Hg(II)) on a contaminated river sediment to bulk adsorption properties. The research involves Hg distribution modeling, as well as measurements of the relative physical availability of the sediment-bound mercury. The work utilizes surface complexation models (SCMs) and bulk partitioning approaches to study and predict trace mercury speciation in the aqueous system, and relates these properties to the physical availability of mercury in the sediments, as quantified by Thermal Programmed Desorption Mass Spectrometry (TPD-MS) (Figure 8 provides a simple schematic of the TPD process). Though a similar pyrolytic technique has been used to study the speciation of mercury in sediments (Biester et al., 2002; Biester and Scholz, 1997), this is the first time that this analytical approach has been used to study the physical availability of mercury. TPD-MS is used throughout this project to determine where and to what degree inorganic mercury is bound in complex contaminated sediment samples, and to identify differences in mercury binding between sediment components (e.g. mercury binding to clay minerals versus mercury binding to organic matter). Finally, TPD-MS is used to semi-quantitatively determine the release energy (energy required to release Hg both from the entire sediment as well as from the individual sediment components (Nicholl and Talley, 2004, Talley et al., 2004).

This EMSI research is being conducted as a collaboration between University of Notre Dame and DuPont Engineering Technology, and EMSI sponsors a graduate student internship program for graduate students to work with

researchers at DuPont for an extended period of time. This project is innovative in that it combines a mechanistic surface complexation approach, an empirical engineering approach (bulk partitioning), and a micro-scale analytical and modeling technique (TPD-MS) to provide an accurate and useful assessment of the distribution and physical availability of inorganic mercury in contaminated sediments. The collaboration of academic and industry researchers provides a unique educational perspective and serves as a template for future industry-academia joint ventures in environmental molecular science and engineering research.

EDUCATION AND OUTREACH

The Environmental Molecular Science Institute at University of Notre Dame is not only a center of research activities, but also serves as a focus for a range of innovative education and outreach programs. In addition to the following ongoing projects, the EMSI also sponsors a variety of other education and outreach activities, such as middle-school science fair mentoring and offering tours and discussion sessions with visiting school groups. The common theme in all Institute outreach activities is to promote an understanding of the importance of environmental molecular science to as wide an audience as possible.

1) Graduate Student Training and Education

One of the primary educational functions of the EMSI is to provide outstanding training of graduate students in environmental molecular science. Toward this end, the Institute awards 12 Institute fellowships to graduate students at University of Notre Dame. The fellowships not only provide stipend support, but they also provide research and training expenses, and enable graduate student recipients to travel to conferences and for research purposes. Institute fellowships are a crucial part of the success of the EMSI because they provide graduate students with research independence from previously-funded projects run by a single advisor. Institute fellows can pursue interdisciplinary research that taps into the expertise of a number of Institute scientists and they can utilize a range of analytical, experimental, and theoretical approaches. The Institute also provides financial support for graduate students to conduct internships both with national laboratory partners as well as with colleagues at DuPont Engineering Technology. These internships enable Institute graduate students access to facilities and expertise at these institutions, but they also provide complementary perspectives on environmental molecular science research.

2) High School Outreach Research Program

The EMSI at University of Notre Dame has initiated a high school outreach research program, in which talented high school students from area schools participate in EMSI research with Institute scientists at Notre Dame. EMSI faculty identify a range of relatively short-term projects that do not require specialized training (other than a standard laboratory safety course and individualized instruction). Research areas include: geomicrobiology, environmental mineralogy pertaining to actinide transport, environmental engineering, groundwater hydrology, and environmental geochemistry. Each year up to nine students (approximately 50% have been female) from three local high schools conduct research in EMSI facilities during the academic year, mentored by EMSI faculty members and graduate students. The high school students present their findings at the annual Indiana Regional Science Fair. In 2004, four high school students who participated in the EMSI Outreach program won science fair prizes, including two 1st places in the Chemistry Division.

The high school research initiative not only serves as an outstanding opportunity for high school students to sample the excitement of scientific research, but it also offers opportunities for the Institute to reach a broader audience concerning the role of molecular science in the study and remediation of the environment.

3) REU and RET Programs

Each summer, the EMSI runs a 10 week Research Experience for Undergraduates (REU) program and a Research Experience for Teachers (RET) program. Typically 8-10 undergraduate students and 2-3 local school teachers participate. Student applicants come from across the country, with typically approximately 10-15 applicants for every available summer research position. The average GPA of program participants is over 3.7 on a 4.0 scale, and college majors of the participants include chemistry, geological engineering, environmental engineering, environmental geosciences, and civil engineering. The summer program concludes each year with a research forum in which each student and teacher participant gives a conference-type presentation, followed by a question-and-answer session. We assess the success of the program by tracking student involvement in science, and through surveys, and each year most participants find the REU to be a positive factor in their decision to further their education and work in science.

SUMMARY

The impact of the Environmental Molecular Science Institute at University of Notre Dame is both scientific and educational. The integration of approaches and disciplines represented in the institute is producing uniquely quali-

fied scientists who are not only educated in advanced molecular-scale research approaches, but who also can use their multi-disciplinary backgrounds to attack current problems in environmental molecular science. The educational and outreach programs run by the EMSI help to educate K-12 teachers and students about the scientific frontiers being explored by Institute researchers. The research conducted at the Institute will markedly increase our understanding of the molecular-scale processes that control the environmental mobility and fate of U, Np, Cd, Cu, Hg, and Pb. This newfound understanding will improve the accuracy of our current geochemical models of contaminant transport, thereby improving our ability to design remediation approaches for contaminated groundwater systems and to better constrain the behavior of nuclear waste products in a repository setting.

References

- Ams, D.A., Maurice, P.A., Hersman, L.E., and Forsythe, J.H. (2002) Siderophore production by *P. mendocina* in the presence of kaolinite: evidence for bacterial responses to Fe stress. *Chemical Geology* 188, 161-170.
- Anthony, C., Pullin, M.J., and Maurice, P.A. (2005, submitted) Effects of Fe on the molecular weight distribution, light absorption, and fluorescence properties of natural organic matter.
- Bethke, C.M. and Brady P.V. (2000) How the K_d approach undermines ground water cleanup. *Ground Water* 38, 435-443.
- Biester, H., Scholz, C.. (1997) Determination of mercury binding forms in contaminated soils: Mercury pyrolysis versus sequential extraction. *Environ. Sci. Technol.* 31, 233-239.
- Biester, H., Muller, G., Scholer, H.F. (2002) Binding and mobility of mercury in soils contaminated by emissions from chlor-alkali plants. *Sci. Total Environ.* 284, 191-203.
- Borrok, D., Fein, J.B., and Kulpa, C.F. (2004) Proton and Cd sorption onto natural bacterial consortia: Testing universal adsorption behavior. *Geochim. Cosmochim. Acta* 68, 3231-3238.
- Borrok, D., Fein, J.B., and Turner B.F. (2005) A universal surface complexation framework for modeling proton binding onto bacterial surfaces in geologic settings. *Amer. J. Sci.* 305, 826-853.
- Boyanov, M.I., Kelly, S.D., Kemner, K.M., Bunker, B.A., Fein, J.B., and Fowle, D.A. (2003) Adsorption of cadmium to *Bacillus subtilis* bacterial cell walls: a pH-dependent X-ray absorption fine structure spectroscopy study. *Geochim. Cosmochim. Acta* 67, 3299-3311.
- Burns, P.C. (2005): U^{6+} minerals and inorganic compounds: Insights into an expanded structural hierarchy of crystal structures. *Canadian Mineralogist* (in press).
- Burns, P.C., Hughes Kubatko, K.-A., Sigmon, G., Fryer, B.J., Gagnon, J.E., Antonio, M.R., and Soderholm, L. (2005): Actinyl peroxide nanospheres. *Angewandte Chemie International Edition* 44, 2135-2139.
- Cabaniss, S.E., Zhou, Q., Maurice, P.A., Chin, Y.-P., and Aiken, G.R. (2000) A log-normal distribution model for the molecular weight of aquatic fulvic acids. *Environ. Sci. Technol.* 34, 1103-1109.
- Cygan, R.T. (2001) Molecular modeling in mineralogy and geochemistry. In R.T. Cygan, and J.D. Kubicki, Eds. *Reviews in Mineralogy and Geochemistry: Molecular Modeling Theory: Applications in the Geosciences*, p. 1-35. The Geochemical Society, Washington D.C.
- Fein, J.B., Bolly, J.-F., Yee, N., Gorman-Lewis, D., and Turner, B.F. (2005) Potentiometric titrations of *Bacillus subtilis* cells and a comparison of modelling approaches. *Geochim. Cosmochim. Acta* 69, 1123-1132.
- Forbes, T.Z., and Burns, P.C. (2005) Structures and syntheses of four Np^{6+} sulfate chain structures: Divergence from U^{6+} crystal chemistry. *Journal of Solid State Chemistry* 3445-3460.
- Forbes, T.Z., Burns, P.C., Soderholm, L. & Skanthakumar, S. (2006): The crystal structures and magnetic properties of $NaK_3(NpO_2)_4(SO_4)_4(H_2O)_2$ and $NaNpO_4SO_4H_2O$: Cation-cation interactions in a neptunyl sulfate framework. *Chemistry of Materials* (submitted).
- Francis, A.J., Gillow, J.B., Dodge, C.J., Harris, R., Beveridge, T.J., and Papenguth, H.W. (2004) Uranium association with halophilic and non-halophilic bacteria and archaea. *Radiochim. Acta* 92, 481-488.
- Frost, P.C., Maurice, P.A., and Fein, J.B. (2003) The effect of Cd on fulvic acid adsorption to *B. subtilis*. *Chemical Geology* 200, 217-224.
- Gorman-Lewis, D., Fein, J.B., Soderholm, L., Jensen, M.P., and Chiang, M.-H. (2005a) Experimental study of neptunyl adsorption onto *Bacillus subtilis*. *Geochim. Cosmochim. Acta* 69, 4837-4844.
- Gorman-Lewis, D., Elias, P.E., and Fein, J.B. (2005b) Uranium adsorption onto *Bacillus subtilis* bacterial cells. *Environ. Sci. Technol.* 39, 4906-4912.
- Gorman-Lewis, D., Fein, J.B., and Jensen, M.P. (2005c, submitted) Enthalpies and entropies of proton and cadmium adsorption onto *Bacillus subtilis* bacterial cells from calorimetric measurements. *Geochim. Cosmochim. Acta*.
- Hennig, C., Panak, P.J., Reich, T., Rossberg, A., Raff, J., Selenska-Pobell, S., Matz, W., Bucher, J.J., Bernhard, G., and Nitsche, H. (2001) EXAFS investigation of uranium(VI) complexes formed at *Bacillus cereus* and *Bacillus sphaericus* surfaces. *Radiochim. Acta* 89, 625-631.
- Hepinstall, S., Turner, B., and Maurice, P.A. (2005, in press) Effects of siderophores on Cd and Pb adsorption to kaolinite. *Clays and Clay Minerals*.
- Johnson, K.J., Cygan, R.T., and Fein J.B. (2005, submitted) Molecular simulations of metal adsorption to bacterial surfaces. *Geochim. Cosmochim. Acta*.
- Kelly, S.D., Boyanov, M.I., Fein, J.B., Fowle, D.A., Yee, N., and Kemner, K.M. (2002) X-ray absorption fine structure determination of pH-dependent U-bacterial cell wall interactions. *Geochim. Cosmochim. Acta* 66, 3855-3871.
- Koretsky C. (2000) The significance of surface complexation reactions in hydrologic systems: A geochemist's perspective. *J. Hydrol.* 230, 127-171.
- Kreller, D.I., Turner, B.F., Namjesnik-Dejanovic, K., and Maurice, P.A. (2005, in press). A comparison of the effects of sonolysis and gamma radiolysis on dissolved organic matter. *Environ. Sci. Technol.*
- Lieser, K. H. and Hill, R. (1992) Hydrolysis and Colloid Formation of Thorium in Water and Consequences for its Migration Behaviour - Comparison with Uranium. *Radiochim. Acta* 56, 37.
- Manecki, M., Maurice, P.A., and Traina, S.J. (2000) Kinetics of aqueous Pb^{2+} reaction with apatites. *Soil Science* 165, 920-933.
- Maurice, P.A., Manecki, M., Fein, J.B., and Schaefer, J. (2004) Fractionation of an aquatic fulvic acid upon adsorption to the bacterium, *Bacillus subtilis*. *Geomicrobiology J.* 21, 69-78.
- Neck, V. and Kim, J.I. (2001) Solubility and hydrolysis of tetravalent actinides. *Radiochim. Acta* 89, 1-16.
- Nicholl, S.I., Talley, J.W. (2005, in press) Development of thermal programmed desorption mass spectrometry methods for environmental applications. *Chemosphere*.
- Panak, P.J., Booth, C.H., Caulder, D.L., Bucher, J.J., Shuh, D.K., Nitsche, H. (2002a) X-ray absorption fine structure spectroscopy of plutonium complexes with *Bacillus sphaericus*. *Radiochim. Acta* 90, 315-321.
- Panak, P.J., Knopp, R., Booth, C.H., Nitsche, H. (2002b) Spectroscopic studies on the interaction of U(VI) with *Bacillus sphaericus*. *Radiochim. Acta* 90, 779-783.
- Pullin, M.J., Progress, C.A., and Maurice, P.A. (2004) Effects of photoirradiation on the adsorption of dissolved organic matter to goethite. *Geochim. Cosmochim. Acta.* 68, 3643-3656.
- Rosenberg, D.A., and Maurice, P.A. (2003) Siderophore adsorption to and dissolution of kaolinite. *Geochim. Cosmochim. Acta* 67, 223-229.
- Sarret, G., Manceau, A., Spadini, L., Roux, J.-C., Hazemann, J.-L., Soldo, Y., Eybert-Berard, L., and Menthonnex, J.-J. (1998) Structural determination of Zn and Pb binding sites in *Penicillium chrysogenum* cell walls by EXAFS spectroscopy. *Environ. Sci. Technol.* 32, 1648-1655.
- Scully, N.M., Lean, D.R.S., McQueen, D.J. and Cooper, W.J. (1995) Photochemical formation of hydrogen peroxide in lakes: Effects of dissolved organic carbon and ultraviolet radiation. *Canad. J. Fish. Aquat. Sci.* 52, 2675-2681.
- Talley, J.W., Ghosh, U., Furey, J.S., Tucker, S.G., Luthy, R.G. (2004) Thermal program desorption mass spectrometry of PAHs from mineral and organic surfaces. *Environ. Eng. Sci.* 21, 647-660.
- Templeton, A.S., Spormann, A.M., Brown, G.E. (2003a) Speciation of Pb(II) sorbed by *Burkholderia cepacia* goethite composites. *Environ. Sci. Technol.* 37, 2166-2172.
- Turner, B.F., Herndon, E.M., and Fein, J.B. (2005a, submitted) Detachment of *Bacillus subtilis* bacterial cells from corundum and hematite surfaces. *Journal of Colloids and Interface Science*.
- Turner, B.F., Herndon, E.M., and Fein, J.B. (2005b, submitted) Effects of pH, ionic strength, and mineralogy on attachment of *B. subtilis* to oxide mineral surfaces. *Colloids and Surfaces A*.
- Ulrich, S.M., Tanton, T.W., Abdrashitova, S.A. (2001) Mercury in the aquatic environment: A review of factors affecting methylation. *Crit. Rev. in Env. Sci. Tec.* 31, 241-293.
- Xiang, X., Huang, Y., Madey, G., Cabaniss, S., Arthurs, L., and Maurice, P. (2005) Modeling the evolution of natural organic matter in the environment with an agent-based stochastic approach. *Natural Resources Modeling Journal*, in press.
- Yee, N. and Fein, J.B. (2001) Cd adsorption onto bacterial surfaces: A universal adsorption edge? *Geochim. Cosmochim. Acta* 65, 2037-2042.
- Young, K., Docherty, K., Maurice, P.A., and Bridgham, S. (2005) Effects of bacterial consortia on natural organic matter degradation. *Hydrobiologia* 539, 1-11.
- Young, K.C. Maurice, P.A., Docherty, K., and Bridgham, S.D. (2004) Bacterial degradation of dissolved organic matter from two northern Michigan streams, *Geomicrobiol. J.* 21, 521-528.



BOOK REVIEW

Micro- and Mesoporous Mineral Phases

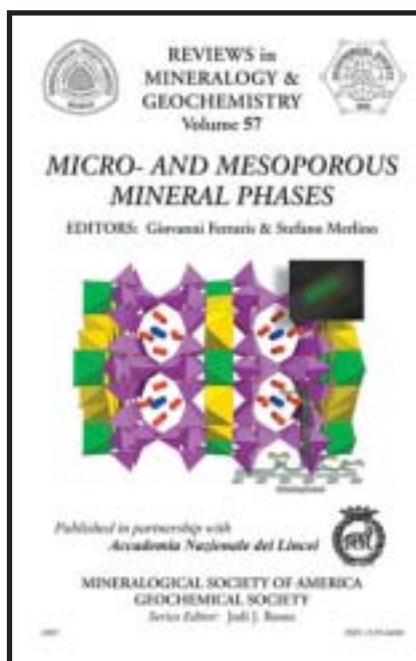
Reviews in Mineralogy and Geochemistry, Volume 57

Giovanni Ferraris and Stefano Merlino, editors

Most geoscientists probably use the term *zeolites* as a synonym for micro- and mesoporous mineral phases. Why then has a new volume with just this title been published only four years after Vol. 45 "Natural Zeolites: Occurrence, Properties, Applications" appeared in the same review series RIMG?

A *zeolite* mineral is, according to the commission of the International [Coombs et al., (1997) *Canad. crystalline substance with a dimensional framework of linked contains open channels and cages occupied by H₂O molecules and (guests). Within the last two considered materials with hosts other than tetrahedra (triangles, micro- and mesoporous materials. present Vol. 57 is much wider than were not treated in the present 2001 is still up to date.*

Although geoscientists are crystalline substances with contain non-tetrahedral building micro- and mesoporous materials, minerals is responsible for many of their geochemical and mineralogical properties. Therefore, the present review is very timely and should serve to make geoscientists aware of the important properties of such poroate minerals.



definition recommended by a Mineralogical Association (IMA) Mineral. 35, 1571-1606], a structure characterised by a 3-[TO₄] tetrahedra (the *host*) that (*pores*), which are usually extra-framework cations decades, some researchers have built from linked polyhedra pyramids, octahedra etc.) to be Consequently, the scope of the that of Vol. 45. In fact, zeolites volume because their review of

unaccustomed to regard inorganic host frameworks that units (so-called poroates) as the porous character of such

In agreement with the recent recommendation of the International Union of Pure and Applied Chemistry (IUPAC) [McCusker et al., (2003) *Micropor. Mesopor. Mater.* 58, 3-13], the present Vol. 57 treats all kinds of poroates, independent of the building units of their inorganic host frameworks and of the dimensionality of their hosts and their pores. Because the properties of poroates depend not only on the structure, but also on the chemical composition of their hosts, the materials covered range from oxides to sulfides and selenides, from silicates to phosphates and uranates, etc. Of the vast number of poroates covered in this volume, the majority are natural minerals but, laudably, related synthetic phases are also discussed. Altogether a wealth of information is given.

The first chapter by L.B. McCusker describes the IUPAC nomenclature and its application to non-zeolite microporous mineral phases, and Chapter 2 by S. Krivovichev deals with the general topology of microporous structures. In Chapter 3, G. Ferraris and A. Gula discuss several families of layer silicates such as the sepiolite - palygorskite family, the astrophyllite group and the bafertisite group as polysomatic

series. In Chapters 4 and 5, N.V. Chukanov and I.V. Pekov present detailed information on the structure, genesis and properties of so-called heterosilicates, i.e., silicates in which silicate anions are complemented by penta-coordinated or octahedrally coordinated transition element cations to form mixed frameworks, which are often microporous. Such minerals are typically formed in postmagmatic processes of peralkaline rocks such as the pegmatites, hydrothermalites and metasomatites from Ilmaussaq, Mount-Saint Hilaire and Lovozero. They can be used as index minerals in the geochemistry of the rare and transition elements and as indicators for specific geological conditions. Other microporous mixed tetrahedral-pentahedral-octahedral framework silicates, their properties and application in catalysis, sorption and luminescence are treated by J. Rocha and Z. Lin in Chapter 6.

Sodalite and the minerals of the cancrinite - davyne group contain cage-like pores but no channels. They were, therefore, not treated in the zeolite volume but are discussed in Chapters 7 and 8 of the present volume, which are written by W. Depmeier and E. Bonaccorsi & S. Merlino, respectively. The latter chapter contains, in addition, a description of the calcium silicate hydrates.

Chapter 9 by M. Pasero deals with tunnel structures. Their hosts are entirely built by linkage of octahedra that are usually centred by transition element cations. The presence of these cations in two different oxidation states requires charge balance by alkali- and alkaline-earth cations located in straight channels (the so-called tunnels). Although minerals of the apatite family are usually considered as dense phases with isolated $[\text{PO}_4]$, $[\text{AsO}_4]$, $[\text{SiO}_4]$, etc. tetrahedra, T. White, C. Ferraris, J. Kim and S. Madhavi describe them in Chapter 10 to have microporous host frameworks built from tetrahedra and octahedra, which are centred by Ca^{2+} , Sr^{2+} , Ba^{2+} , Pb^{2+} , etc. Channels within the framework also contain these cations and F, OH^- or O^{2-} anions.

In Chapter 11, E. Makovicky explains that a large number of sulfides and selenides of cations with a lone electron pair, such as As^{3+} , Sb^{3+} , Bi^{3+} , Pb^{2+} etc., have microporous hosts with channels occupied by cations and sometimes anions. The final chapter, written by M. Mellini, reports on microporous forms of carbon (anthracites, fullerenes and carbon nanotubes), serpentines and clathrate hydrates.

The volume is a comprehensive and richly illustrated review of micro- and mesoporous crystalline phases with inorganic host structures (poroates). It is well edited and produced. Geochemical aspects are particularly addressed in Chapters 4 and 5 and to a lesser extent in Chapters 8, 10 and 11. Their technical applications as ion exchangers, absorbers, catalysts, fuel-cell electrolytes, luminophores and for waste disposal are discussed in Chapters 4, 6, 8-10, and 12. The review is especially suited to widen the horizon of geochemists and mineralogists alike with respect to correlations between structure and properties of minerals.

The usefulness of this, as well as other volumes of RiMG, would be improved if at the end there would be an index of the minerals described. With present day computer programs this should not be a difficult task.

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Center for Environmental Kinetic Analysis: *Biogeochemists spanning scales of space and time*

Philosophy

After four and a half billion years, the Earth's surface remains far removed from chemical equilibrium. The interaction between the lithosphere and the biosphere is especially pertinent in the study of dynamic geochemical cycles. Therefore, researchers must focus on the kinetics and rates of biogeochemical reactions and on the physical and chemical feedbacks that influence biogeochemistry across a range of scales.

The Center for Environmental Kinetics Analysis (CEKA) at Penn State has begun an ambitious effort to synthesize the kinetics of biogeochemical reactions for both pristine and anthropogenically perturbed systems. Given the difficulty of extrapolation of chemical kinetics from small laboratory scales to larger field scales, CEKA's task represents a first-order philosophical and practical challenge. Is the complexity that underlies natural systems inherently irreducible, or is it possible to dissect geochemical cycles into parts that can be integrated to produce a model of surficial chemistry with predictive capability? Scientists at CEKA argue that training new scientists to transect multiple length scales and chemical systems offers the best hope of determining the way in which molecular scale behavior can be analyzed to increase understanding and predictability of the macroscopic world (Fig. 1).

The Center for Environmental Kinetic Analysis (CEKA) is an Environmental Molecular Sciences Institute (EMSI) based at Penn State with members at three National Laboratories (Sandia, Lawrence-Berkeley, and Pacific Northwest National Laboratories). CEKA is a joint research and education initiative of the National Science Foundation (NSF), the U.S. Department of Energy (DOE), and Penn State University. Funding for Penn State faculty and students is provided by the NSF Divisions of Chemistry and Earth Sciences under the Environmental Molecular Science Institute Program (EMSI). DOE partners are supported by the DOE Office of Science, Division of Environmental Remediation Sciences.

CEKA brings together chemists, geochemists, biochemists, soil scientists, materials scientists and engineers to measure and synthesize kinetic data for environmental systems and to model the temporal evolution of such systems. The Center's initiative emphasizes the problem of scaling in terrestrial environmental kinetics, with especial emphasis on the mineral-water interface with and without cells and biofilms. In a highly collaborative research effort, CEKA focuses on the following question:

What approaches and insights can be developed to extrapolate rates of environmentally important reactions across a variety of scales?

Current Research at CEKA

CEKA is organized into four research groups with overlapping interests: the Dissolution Interest Group, the Precipitation Interest Group, the Bioreaction Interest group, and the Synthesis Interest Group. Graduate students work within each interest group at a variety of scales. Postdoctoral scholars work across the Interest Groups by spearheading cross-cutting approaches. This interwoven infrastructure is already resulting in a variety of interdisciplinary approaches to CEKA's ambitious objectives.

The Dissolution Interest Group

The Dissolution Interest Group (DIG) focuses its efforts on geochemical dissolution reactions at different scales. A quantitative understanding of dissolution reactions is critical in the understanding of the fate and transport of substances in the environment. The group uses a variety of methods including NMR, atomic force microscopy, and computer-facilitated spatial modeling of reaction kinetics to achieve its goals.

Three questions focus the DIG's research:

- What are the important controls on abiotic dissolution of Fe (and Mn) oxides and how do these processes depend on the intrinsic reactivities of hydrated Fe (and Mn) oxide surfaces?
- How can we use experimental and computational tools to predict reactive surface area across spatial scales?
- How can we understand and relate the rates of dissolution of a mineral phase, either alone or in the presence of porous media, measured in reactors at different scales?

Of particular current interest is the recent work spearheaded by CEKA faculty members Karl Mueller (Dept of Chemistry) and Sue Brantley (Geosciences) to quantify and model reactive surface area and its development. In comparing the development of plagioclase reaction fronts in three soils in the United States to fronts modeled using laboratory-derived weathering rates in the reactive transport code FLOTRAN (written by Peter Lichtner, Los Alamos National Laboratory), graduate student Joel Moore noted that weathering is consistent with a decrease in reactive surface area over time (Fig. 2).

Because no method to measure reactive surface area is available, Mueller and graduate students developed a new spectrographic technique that employs the covalent attachment of a fluorosilane molecule to hydroxyl groups in rhyolitic and dactic glasses. ^{19}F -NMR is used to quantify the reactive OH groups after surface modification. The results are promising, showing good correlation between reaction rate and reactive site density for naturally weathered volcanic glasses. Cross-polarization magic-angle spinning NMR investigations of Q-site speciation and *ab initio* predictions of ^{29}Si shifts will ultimately be combined with ^{19}F and ^{29}Si NMR analyses of silane-modified samples to quantify the reaction rates as a function of reactive surface site evolution (Mueller et al., 2005). The NMR work is complemented by molecular-scale modeling to determine the activation energies for Si hydrolysis reaction pathways (e.g. Criscenti et al., 2005) in order to understand how connectedness of Si atoms affects silicate dissolution.

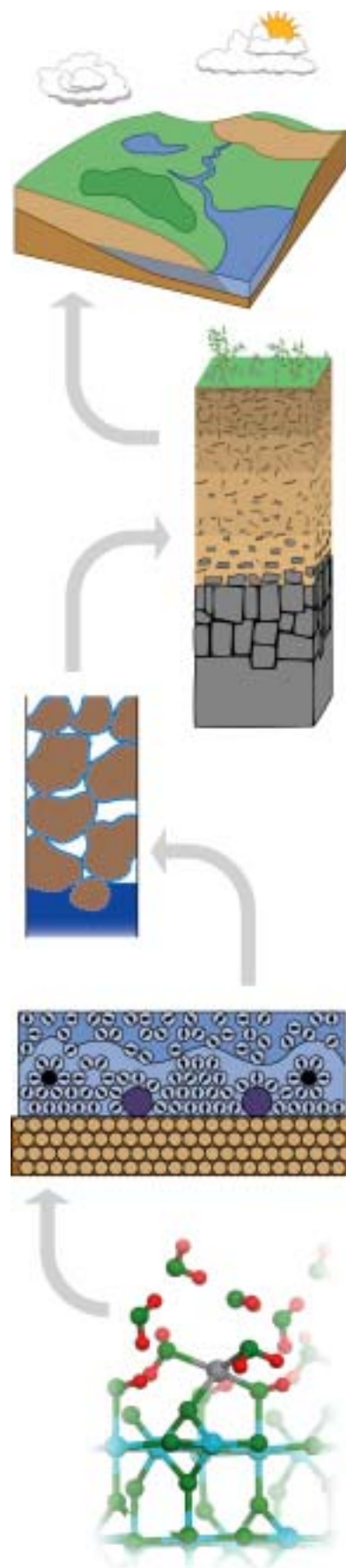
Stochastic simulations developed by CEKA postdoc Joel Bandstra (Bandstra et al., 2005) reveal the changes in reactive site density and distribution that occur through dissolution reactions. By combining theory-driven models and stochastic approaches, CEKA scientists are working towards the identification and quantification of scaling laws between surface area and reactivity (Fig. 2).

The Precipitation Interest Group

The Precipitation Interest Group is quantifying the kinetic rates and mechanisms of biogeochemical precipitation reactions. Methodologies now used in CEKA include time-resolved X-ray diffraction, size exclusion chromatography, powder X-ray and neutron diffraction, NMR, 2D-gel electrophoresis, and transmission electron microscopy.

The four questions that are the motivation for the Precipitation Group's research are:

Figure 1. CEKA works across scales, developing biogeochemical models that transcend the constraints of bench-top experimentation. A strong interdisciplinary emphasis within CEKA enlists the cooperation of theorists, modelers, and experimentalists in chemistry, molecular biology, material science, and the geosciences to investigate some of today's most challenging biogeochemical questions.



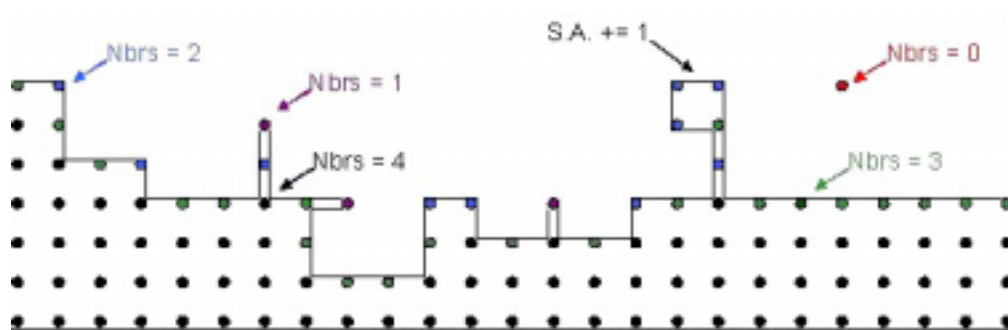


Figure 2. Stochastic modeling of reactive surface evolution. Both the reactivity and microscopic area of a dissolving surface depend on the distribution of surface sites. Since every dissolution event causes a change in the distribution of sites (shown here as a schematic surface with the number of neighbors, *Nbrs*, identified for characteristic sites), it should be possible to derive coupled rate equations for reactivity and surface area. In this work we employ stochastic simulations of dissolution with the goal of finding universal scaling laws between surface area and reactivity.

- What controls homogeneous nucleation and growth of simple one-component metal oxides?
- What factors control the nucleation, growth, and transformation of mixed Fe, Al- and Si- oxides from solution (homogeneous growth) and on mineral surfaces (heterogeneous growth)?
- What factors control the transformation of Fe ± Si ± Al oxides interacting with water over time?
- How can we understand and predict the rates of coupled dissolution and precipitation of various phases, either alone or in the presence of porous media, measured at different scales within and in the absence of a porous medium?

The Precipitation Interest Group members tackle these research questions in the field, in the laboratory, and with *ab initio* models. For example, the research group led by Dr. Peter Heaney (Geosciences) is studying biologically-driven reactions that can alter precipitate minerals. Many of the bacterial species that engage in dissimilatory Fe reduction also can reduce Mn in minerals such as birnessite [$\text{Na}_{0.58}(\text{Mn}^{4+}_{1.42}, \text{Mn}^{3+}_{0.58})\text{O}_4 \cdot 1.5\text{H}_2\text{O}$], which is common in soils and sediments. Heaney's research group has observed the reduction of birnessite into rhodochosite (a manganese carbonate) by the membrane fraction of bacterial cultures using synchrotron X-ray diffraction. The clarity of the results of this experiment suggests that high resolution kinetic studies of biologically mediated reactions may succeed using this novel technique.

The Bioreaction Interest Group

Microorganisms facilitate both precipitation and dissolution in the subsurface environment. Under the leadership of Ming Tien, the Bioreaction Interest Group (BIG) examines the role, mechanisms, and rates of bioreaction at different scales using a broad combination of techniques. 2D-gel electrophoresis and bioreactors help quantify biotically-facilitated metal reduction. Atomic force microscopy is used to measure biofilm adhesion to mineral substrates.

The Bioreaction group pursues answers to four key questions:

- How do molecular characteristics determine the kinetics of biofilm attachment and growth on mineral surfaces and can bioadhesion measurements made at molecular scales be used to predict adhesion and reactivity at macroscopic (column) scales?
- What controls the nucleation, transformation, and growth of Fe minerals during bioreaction?
- Can we scale from the kinetics of dissimilatory iron reduction with isolated enzymes to cultures?
- How can a molecular-scale mechanistic understanding of bacterial enzymatic reduction of solid-phase iron(III) oxides be up-scaled to predict and model biological iron(III) reduction at larger scales?

In order to understand the biogeochemistry of dissimilatory Fe reduction, Ruebush et al. (2005a and b) have examined the physiology of iron reduction by *Shewanella*, a facultative anaerobic bacterium, known for its ability to use insoluble Fe and Mn as electron acceptors. Proposed mechanisms for Fe reduction include the utilization of an exogenous electron shuttle, direct contact of the bacterium with the substrate, and chelation of $\text{Fe}^{3+}_{(\text{aq})}$. In an effort to understand the role of *Shewanella* membrane proteins in Fe reduction via direct contact, Ruebush et al. (2005a) investigated the role of membrane fractions (outer, cytosolic, and total) in the reduction of ferric iron in solution and of Fe(III) in goethite. Goethite reduction was observed to be most pronounced in the presence of fragments of the total membrane, suggesting that kinetic interactions involving both the outer and cytosolic membranes are necessary for dissimilatory iron reduction.

The Synthesis Interest Group

This interest group works towards transforming CEKA's laboratory and theoretical results into easily accessible and readily applicable information, thereby enabling CEKA to have both powerful scientific and educational impacts, and to have broad-reaching applications and audiences. The broad reach of this interest group is exemplified by its three consensus questions:

- Can measurements of mineral-water reactions at laboratory scales be used to predict mineral-water reactions in a field site?
- How can we implement the collection, collation, and synthesis of environmental kinetics data into useable databases for dissemination to the broader community?
- How can high quality 3D visualizations be used to provide insight into the factors controlling environmental kinetics and to communicate this information to a range of audiences?

To address these three questions, the Synthesis Interest Group focuses on a field site, on kinetics databases, and on the GeoWall as a visualization tool. CEKA recently identified a field site to begin investigations of weathering rates and redox reactions. Shale Hills Experimental Watershed, 20 miles from Penn State University, has been the site of ongoing hydrological research (Duffy, 1996; Lin et al., 2005). The established hydrologic database will greatly facilitate CEKA's efforts to apply data developed through modeling and empirical investigations to the field. The site will be used for both research and educational efforts for the Penn State community.

CEKA postdoc Joel Bandstra is compiling and synthesizing kinetics data for mineral dissolution and metal reduction reactions. As part of a separately funded NSF Cyberinfrastructure project, Bandstra, along with Penn State's School of Information Science and Technology faculty members Prasenjit Mitra and C. Lee Giles, is developing an online resource of kinetic reaction data that can be accessed and used freely by the scientific community.

CEKA Outreach and Visualization Specialist Chuck Anderson introduced both a permanent and a mobile Geowall 3D visualization station at Penn State. He uses the mobile unit for presentations on campus, at K-12 activities, and at national meetings such as the American Chemical Society National Meeting in Washington D.C. in August 2005. Students in CEKA are required to incorporate GeoWall 3D-visualizations of their data as a part of their research. The GeoWall has already been used by CEKA members to visualize CAT-scan data of weathering rinds on rocks (Fig. 3, image made by CEKA graduate student Alexis Navarre and Chuck Anderson), to visualize data from 2D-gel electrophoresis, and to visualize specific conductivity in subsurface contaminant plumes.

Opportunities at CEKA

Outreach

CEKA delivers public outreach through museum exhibits, K-12 outreach through teaching modules, and professional outreach through short courses. CEKA collaborators Dr. Peter Lichtner of Los Alamos National Lab and Dr. Carl Steefel of Lawrence Berkeley National Lab will offer a short course in reactive transport May 11-13, 2006.

Undergraduate

A summer Research Experience for Undergraduates (REU) program places students in the laboratories of CEKA faculty and offers opportunities for participating in hands-on biogeochemical research.

Graduate Students

CEKA currently has funding available for doctoral students who have strong interests in the study of environmental biogeochemistry in an interdisciplinary environment. Doctoral students receive a generous funding package that includes stipend and tuition as well as research and travel support. The planned stipend and tuition support is for multiple years; single year packages are also available. Doctoral students enter the program through one of seven departments (Biochemistry and Molecular Biology, Chemistry, Civil and Environmental Engineering, Crop and Soil Sciences, Energy and Geo-Environmental Engineering, Geosciences, Materials Science and Engineering), or the Intercollege Program in Materials.

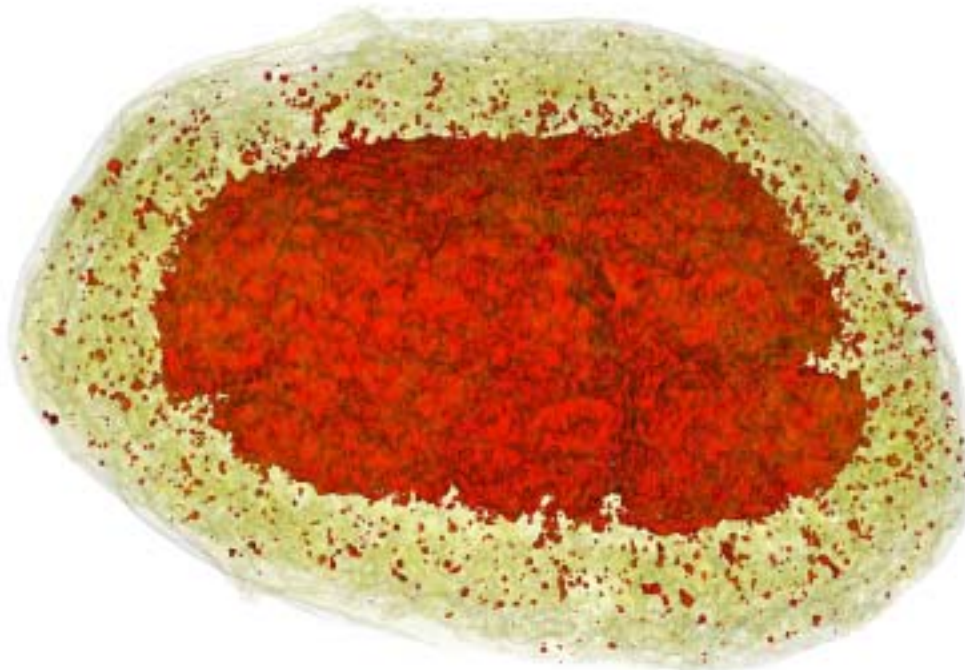


Figure 3. Sections of a weathered basalt clast were obtained by Alexis Navarre through CAT scan imaging. Using the CAT scan data, Chuck Anderson, CEKA's GeoWall innovator, was able to generate 3-dimensional imagery of the internal density patterns of the clast revealing a distinctive weathering rind around a fractured, but dense basalt core. On the GeoWall, this image can be rotated freely and viewed in three dimensions. The yellow region is the weathering rind. The red volumes represent regions of material that are above a threshold density. Visualization of the manually determined threshold density can be adjusted to reveal spatial patterns in weathering.

Postdocs

The Center for Environmental Kinetics Analysis also offers opportunities for postdoctoral scholars interested in investigating biogeochemical kinetics using experimental, theoretical, and field techniques.

Contacting CEKA

Please visit our website (www.ceka.psu.edu) or contact Denise Kowalski at ceka@psu.edu for more information.

References

- Joel Z. Bandstra, Paul G. Tratnyek, Susan L. Brantley. Relating the kinematics and the dynamics of reacting surfaces. 230th ACS National Meeting in Washington, D.C., August 28-Sept 1, 2005.
- Criscenti, L. J., J. D. Kubicki, and S. L. Brantley. 2005. Silicate glass and mineral dissolution: calculated reaction paths and activation energies for hydrolysis of a Q3 Si by H_3O^+ using *ab initio* methods. *Journal of Physical Chemistry A*, 110, 198-206.
- Duffy, C. J. 1996. A two-state integral-balance model for soil moisture and groundwater dynamics in complex terrain. *Water Resources Research* 32: 2421-2434.
- Lin, H.S., J. Bouma, Y. Paschepsky. (ed.). 2005. *Hydropedology: Bridging disciplines, scales, and data*. Geoderma special issue. Elsevier. (*in press*).
- Mueller, K., J. Bandstra, J. Kubicki, L. Criscenti, J. Moore, N. Washton, M. Davis, A.F. White, P. Lichtner, S. Brantley. 2005. New tools and concepts for understanding the evolution of mineral surface area for extrapolation of environmental kinetics. Proceedings, AGU Meeting, San Francisco, CA, December 5-9, 2005.
- Ruebush, S., GA. Icopini, SL. Brantley, and M. Tien. 2005a. *In vitro* enzymatic reduction kinetics of mineral oxides by membrane fractions from *Shewanella oneidensis* MR-1. *Geochimica et Cosmochimica Acta* 70: 56-70.
- Ruebush, S., SL. Brantley, and M. Tien. 2005b. Reduction of mineral oxides by membrane fractions of *Shewanella oneidensis*. Proceedings, ACS National Meetings Washington, D.C. August 29, 2005.



New GS Logo Design Contest Deadline Extended

Submissions accepted through February 28, 2006

Due to a distribution mix-up with the December issue of Elements, the deadline for submitting entries to the GS Logo Design Contest has been extended. We have received a number of terrific entries but want to be sure that all GS members have an opportunity to participate and win.

Announcement that was published in Elements:

If you have been wishing for an opportunity to put your graphic arts creativity to work in a high-impact way, here is your chance! GS has extended the deadline for the contest to submit a new logo for our society! When GS began 50 years ago, our organization adopted the currently used hand-drawn logo. As we look forward to the next 50 years, we are looking to update our widely-used emblem with a fresh look.

What sort of fresh look? Most modern logos or emblems share similar qualities: easy to use in electronic as well as traditional media, simple styles and readily represented in black/white or color formats. The logo should be scalable and not be too detailed so that it works well at low resolution. Logos may include The Geochemical Society or GS somewhere in the design but this is not mandatory. Creativity, originality, aesthetics, use of space and color will all be used in the selection process. Please keep these suggestions in mind while designing your entry.

A cash prize of \$500 USD will be awarded to the winner. Plus the winner will have the pleasure of seeing his/her creative juices displayed by the GS for years to come as our society continues to grow in size and impact.

The Winner will be announced in March 2006. To enter, please send your submission(s) as an electronic file (preferred formats are .eps or illustrator). It would be advantageous to provide your entry in both b/w and color versions. Flash format is also welcome. All entries will be considered and you may make as many submissions as you like.

Send your entries and your contact information directly to gsoffice@geochemsoc.org. The winning entry becomes the property of the Geochemical Society. By submitting an entry, you agree to grant GS exclusive, royalty-free license to use your logo entry for purposes of the contest. The winner will be required to sign a notarized affidavit releasing intellectual rights to the Geochemical Society.

The 1955 logo can be viewed on the GS website at www.geochemsoc.org or on our many publications. If you have questions regarding this contest, please contact Seth Davis at gsoffice@geochemsoc.org.

Goldschmidt 2006

16th Annual V.M. Goldschmidt Conference 2006

27 August – 1 September 2006

Melbourne Exhibition and Convention Centre, Melbourne, Australia

www.goldschmidt2006.org

Conference topics shall highlight important issues, facilitate open discussion and provide fresh perspectives. Please visit the conference website for more details and to register for this not to be missed conference. A program summary is provided below.



Theme 1: Advances in techniques in geochemistry

Trevor Ireland, Andrew Berry

- S1-01: Nuclear methods in geochemistry
- S1-02: Reactions and processes at mineral surfaces and boundaries
- S1-03: Determining coordination and structure with synchrotron light
- S1-04: Techniques for Earthtime and CRONUS
- S1-05: Techniques for isotopic and abundance measurements of light elements
- S1-06: Techniques for heavy stable isotope analysis
- S1-07: Techniques for nanoscale geochemistry
- S1-08: Noble gases in the 21st century

Theme 2: Mineral deposits and ore geochemistry

Andy Barnicoat, Chris Heinrich

- S2-01: Quantitative hydrodynamic and thermodynamic modelling of hydrothermal processes
- S2-02: Fluid-melt-mineral interactions in nature and experiments
- S2-03: Element mobility in the regolith: ore body formation, dispersion and discovery
- S2-04: Geochemical and isotopic techniques – applications to ore deposits and exploration
- S2-05: Sources and mobility of metals across scales: from veins to the lithosphere
- S2-06: Sulfide Mineralogy and geochemistry; to mark the publication of Vol 60 in the Reviews in Mineralogy and Geochemistry series
- S2-07: Geochemistry of Platinum Group Elements and their ores

Theme 3: Solar system formation

Herbert Palme, Marc Norman

- S3-01: Chronology of the early Solar System (including an additional workshop on construction of a time scale for the early solar system)
- S3-02: Stellar and Nebular Processes
- S3-03: Planetary Formation and Differentiation
- S3-04: Geochemistry of Planetary Surfaces
- S3-05: Cosmochemistry of Habitable Planets

Theme 4: Convecting Mantle

Bernie Wood, Janne Blichert-Toft

- S4-01: Experimental constraints on upper mantle processes - a special symposium honouring Prof. David H Green
- S4-02: Messages from the past—the signature of ancient subduction
- S4-03: Early Mantle evolution
- S4-04: Mantle-core interactions
- S4-05: Perovskite and post-perovskite- stability, geochemical and geodynamical consequences
- S4-06: Melting at ridges
- S4-07: Volatiles in the mantle
- S4-08: Plumes and large igneous provinces

See also S5-07

Theme 5: Lithosphere evolution

Roberta Rudnick, Greg Yaxley

- S5-01: The deepest lithosphere and beyond: Diamonds and related research - a session in honour of Jeff W. Harris
- S5-02: Earth Evolution 4.5 to 3.5 Ga: Deciphering the Earliest Global Systems
- S5-03: Geochemical and geophysical probing of continental dynamics
- S5-04: Precambrian ophiolites and greenstone belts: insights into mantle dynamics and lithosphere evolution
- S5-05: Processes of mantle refertilisation and modification
- S5-06: Ross Taylor symposium – celebrating Ross' career and contributions
- S5-07: Shen-su Sun Symposium – Geochemical reservoirs and mantle convection (jointly with theme 4)
- S5-08: Continental Crust Subduction and Recycling
- S5-09: Granites and mantle-crust interaction

Theme 6: Subduction processes

Tim Elliott, Richard Arculus

- S6-01: Fluid loss during early (< 2 GPa) subduction
- S6-02: "Deep" fluid release from the slab
- S6-03: Mantle melting in subduction zones
- S6-04: Unscrambling differentiation
- S6-05: Mineralisation at subduction zones
- S6-06: Subduction zone evolution in 4-D

Theme 7: Geochemical constraints on timescales and mechanisms of tectonic processes

Derek Vance, Joerg Herrmann

- S7-01: Accessory phases and trace elements: links between geochronology and petrology
- S7-02: Up and down: Geochronological constraints on paleotopography and tectonic geomorphology
- S7-03: Fast and furious versus slow and steady: rates of tectonic and magmatic processes
- S7-04: Extreme metamorphism
- S7-05: Light elements in the continental crust
- S7-06: Fault systems: their geochronology and geochemistry

Theme 8: Biogeochemistry and the origin and evolution of life

Malcolm Walter, Mike Russell

- S8-01: Mediation across the abiotic-biotic transition at the dawn of life
- S8-02: Quantum aspects of life
- S8-03: Novel isotopic tracers of biogeochemical processes
- S8-04: Compound specific isotope analysis and its contributions to palaeoreconstruction
- S8-05: Major episodes of extinction, radiation and biogeochemical change
- S8-06: Microbe-mineral interactions
- S8-07: Life's signatures and products up to 2.0 Ga
- S8-08: Possible biogeochemistries of Mars
- S8-09: Timescales of human evolution

Theme 9: Aquatic geochemistry and fluids in the crust

John Mavrogenes, Sue Brantley

- S9-01: Fluid immiscibility in High T systems
- S9-02: Supercritical behaviour
- S9-03: Water-rock interaction in aquifers: reactions, rates, controls
- S9-04: Low-temperature geochemistry in surface environments
- S9-05: Nanoscale size effects on geochemical processes: reactivity, kinetics, and pathways

Theme 10: Surface processes, low temperature systems and landscape evolution

Paulo Vasconcelos, Rod Brown

- S10-01: Geochemistry, chronology and global consequences of terrestrial weathering
- S10-02: Low temperature thermochronometry: models, methods and applications
- S10-03: Terrestrial cosmogenic nuclides: surface process rates and/or dates?
- S10-04: Biogeochemical cycling of elements in the surficial environment
- S10-05: High resolution palaeoclimate chronologies and proxies
- S10-06: Synchrotron applications to environmental mineralogy
- S10-07: Mobility, availability and toxicity of pollutants
- S10-08: Geochemistry of wine

Theme 11: Ocean chemistry and circulation; climate and environment

Rachael James, Malcolm McCulloch

- S11-01: Deep-Sea Carbonate Systems
- S11-02: Marine biogeochemical forcing of Earth's atmosphere on short and long timescales
- S11-03: Ocean chemistry: past, present and future
- S11-04: Geochemical proxies for the past marine environment
- S11-05: Continental input of dissolved material to the oceans: control and fate
- S11-06: Absolute and relative chronologies of climate change

General Symposia

- G-01: Analytical geochemistry
- G-02: Atmospheric geochemistry
- G-03: Biogeochemistry
- G-04: Computational geochemistry
- G-05: Cosmochemistry
- G-06: Crystallography
- G-07: Environmental geochemistry/mineralogy
- G-08: Experimental geochemistry/petrology
- G-09: Geochronology
- G-10: Hydrology/Hydrogeochemistry
- G-11: Hydrothermal geochemistry
- G-12: Igneous geochemistry
- G-13: Isotope geochemistry
- G-14: Marine geochemistry
- G-15: Metamorphic geochemistry
- G-16: Mineral deposits

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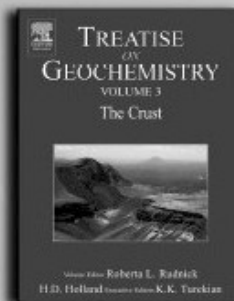
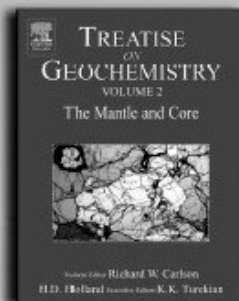
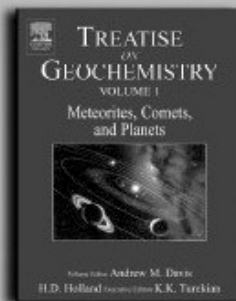
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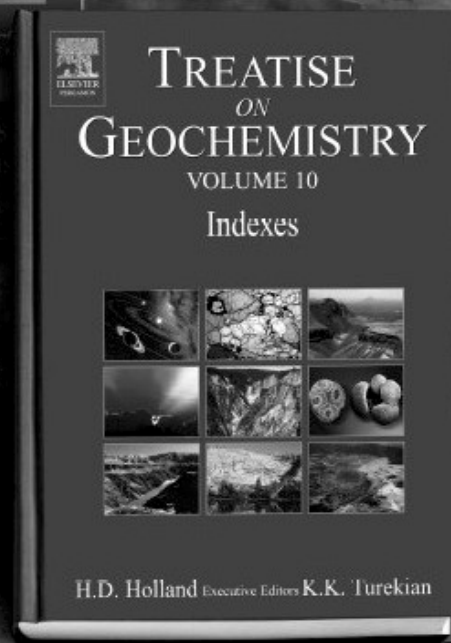
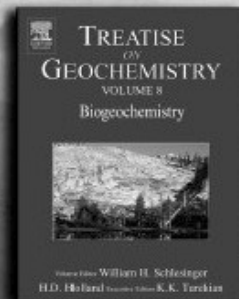
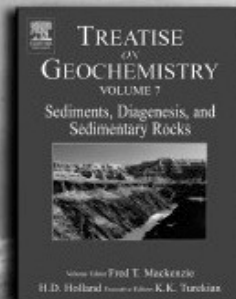
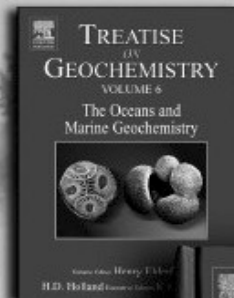
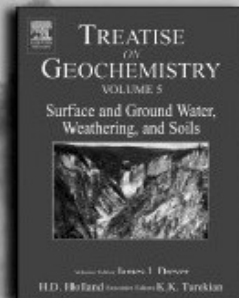
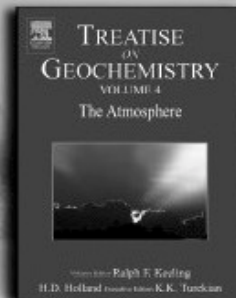
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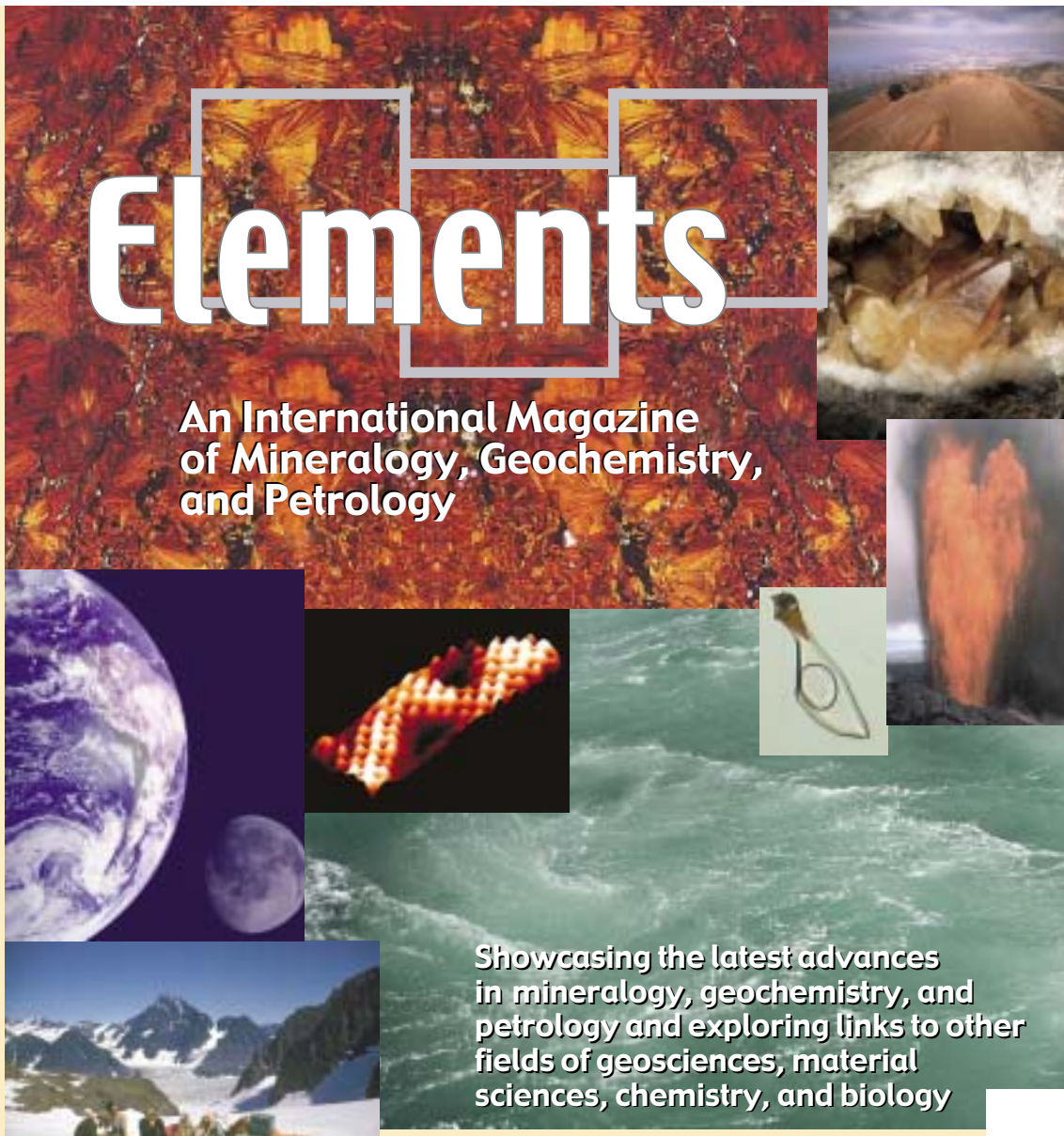


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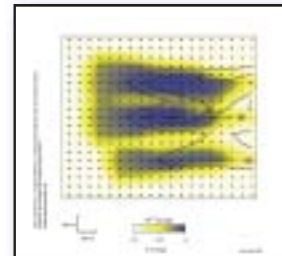
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