



2021 ACS Spring National Meeting
April 5-16, 2021, San Antonio
*Macromolecular Chemistry:
The Second Century*



Geochemistry Division

Call for Abstract Submission

Abstract submission: Dec 16, 2020 – Jan 19, 2021

Meeting time: April 5–16, 2021

Meeting format: Live interactive virtual sessions

General information about the conference can be found at:

<https://www.acs.org/content/acs/en/meetings/national-meeting.html>

You are invited to submit abstracts for the following GEOC symposia:

- 40 Years of High-Resolution NMR Spectroscopy of Inorganic Solids
- Fundamental Reactions Driving Macroscopic Geochemical Processes
- Crystallization Pathways: New Perspectives on Nucleation, Growth & Dissolution of Natural & Synthetic Materials
- Biogeochemical Transformation in the Underground Environment – Natural Processes and Engineered Implementations for Contaminant Abatement
- The Evolution of Macromolecular Carbon through Space and Time
- Interfacial Reactions under Nano-scale Confinement
- Molecular Processes at Mineral-Water Interfaces
- Engineered Nanomaterials and Synthetic Macromolecules in the Environment: Fate, Behavior, and Effects
- Reactivity & Transformation of Manganese Oxides in Natural and Engineering Systems
- Reactive Transport Modeling: A Cutting-Edge Tool for Investigating Coupled Processes
- General geochemistry

Detailed description and contact information for each symposium are attached.

Abstract submission: Please submit your abstracts using the ACS Meeting Abstracts Programming System (MAPS) at <http://maps.acs.org>. Abstracts submission window is **Dec 16, 2020 – Jan 19, 2021**.

Registration fee: \$99 for ACS members, \$149 for non-members, \$29 for students, no cost for unemployed members and 50-year emeritus members.

Questions?

- General information about the conference can be found at:
<https://www.acs.org/content/acs/en/meetings/national-meeting.html>
- For questions about specific symposia, please contact the organizer directly.
- For general questions about the Geochemistry Division symposia and activities, please contact Yuanzhi Tang (yuanzhi.tang@eas.gatech.edu).



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40 Years of High-Resolution NMR Spectroscopy of Inorganic Solids
Co-sponsored by PHYS and INOR

2020 was the 40th anniversary of the publication of the paper “Structural Studies of Silicates by Solid-State High-Resolution Si-29 NMR spectroscopy” by Endel Lippmaa and collaborators (JACS 102, 1980, 4889-4893). It is not an exaggeration to say that this paper is the foundation for the extraordinary contributions that high resolution NMR has made to understanding the structure and dynamical behavior of oxide and related materials since then. It has been cited more than 1,000 times (Web of Science).

This symposium is focused on the development and impact of NMR spectroscopy of inorganic materials since then and on the current developments that are continuing to drive the field. Potential topics include a brief history of high-resolution NMR techniques for solids and its application to inorganic materials as well as NMR studies of ordered and disordered crystalline materials, glasses and other disordered materials, intercalation and ion/fluid exchange materials, nanomaterials, high pressure and temperature materials, paramagnetic materials, cements, and other environmental/geochemical applications.

General information about the conference can be found at: www.acs.org/meetings.
Any other inquiries should be directed to the symposium organizers:

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Fundamental Reactions Driving Macroscopic Geochemical Processes

Chemical reactions occurring geologic environments are driven by heterogeneous molecular- to nano-scale processes. Dynamic variations in composition and structure reflect interactions between mineral surfaces (both ideal and defective) and ions/molecules in solutions confined in geologic media under various temperatures and pressures. Understanding these processes is essential for the interrogation of macroscopic geochemical data, extrapolation of lab-scale experimental data, and creation of quantitative predictive models. This symposium focuses on a fundamental understanding of key geochemical processes in aqueous solutions, at mineral-water interfaces, and within geologic media that affect micro to macroscopic phenomena including mineral nucleation, growth, and dissolution, changes in porosity, permeability, and water quality. We encourage contributions from a broad range of scientific disciplines whose research highlights recent advances in theoretical, computational, and experimental designs that bridge multiple scales of spatial and temporal observations. Topics of interest include, but are not limited to:

- Molecular basis of phase transformations in complex geochemical environments (connecting ion solvation and chemical speciation, crystal nucleation and growth, and solid-state replacement reactions)
- Effect of multi-scale porosity and permeability on the local ionic mobility in highly heterogeneous media
- Multiscale modeling of global reaction rates on solid-fluid interfaces and confinement

General information about the conference can be found at: www.acs.org/meetings.
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Crystallization Pathways: New Perspectives on Nucleation, Growth & Dissolution of Natural & Synthetic Materials

Mineral nucleation, growth, and dissolution are important geochemical processes that occur in a wide variety of natural systems, including bulk solution, solid-liquid interfaces, and confinements. Over the past decade, high-resolution experimental and computational studies have revealed complex pathways of crystal nucleation and growth that do not conform to classical monomer-by-monomer processes. Examples are the formation of metastable, often amorphous, intermediates prior to crystal nucleation and the growth of minerals by particle attachment. A mechanistic understanding of these complex crystallization pathways and associated metastable intermediates is crucial for deciphering the chemical and physical controls on mineral structure and composition.

This symposium seeks contributions from various scientific disciplines that advance the current understanding of mineral nucleation, growth, and dissolution in synthetic and natural environments. We invite observational and experimental contributions that present novel syntheses, structures, mechanisms, and phase transitions, as well as computational efforts to establish and develop the framework needed to describe these phenomena.

Topics of interest include, but are not limited to:

- Classical and non-classical nucleation pathways
- Precipitation/dissolution at solid-liquid interfaces and in confinements
- Precipitation/dissolution of biominerals

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Any other inquiries should be directed to the symposium organizers:

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Biogeochemical Transformation in the Underground Environment – Natural Processes and Engineered Implementations for Contaminant Abatement
Co-sponsored by ENVR

Biogeochemical transformation of redox labile elements (e.g., C, N, S, Fe and Mn) has a great impact on electron transport, cycling of nutrients, and contaminant sequestration or attenuation. A significant portion of these processes occur in the aquatic environment, including subsurface systems near redox boundaries where abundant interactions among aqueous, biological, and mineral entities arise enabling electron flow via coupled biological and geochemical reactions.

Although significant advances have been made in understanding the fundamentals of the dominant biogeochemical processes, the impacts of these natural processes on the transformation of contaminants on a societally relevant time scale represent a new challenge that is critical to address. Applied questions such as whether engineered measures can be used to stimulate desired geochemical processes or vice versa for sustained environment restoration remain largely open.

This symposium invites discussion on recent advances in various aspects of the field, including but not limited to the following topics:

- Electron transfer at bio-carbon or bio-mineral interface
- Impacts of biogeochemical cycling on the speciation and mobility of trace elements
- Impact of flooding and changes in water chemistry on soil contaminant and nutrient mobility
- Transformation or attenuation of organic electron donors, including anthropogenic chemicals as well as natural organic matter
- Production of reactive oxygen species via coupled biological and abiotic processes
- Methods for laboratory or field characterization of geochemical conditions or indicators of biological processes
- Prediction of intermediate- and long-term subsurface reactive capacity and kinetics based on instantaneous or short-term laboratory or field measurements

General information about the conference can be found at: www.acs.org/meetings.
Any other inquiries should be directed to the symposium organizers:

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The Evolution of Macromolecular Carbon through Space and Time

Macromolecular carbon (MMC) is ubiquitous in our solar system and has been identified and characterized in a wide variety of materials including carbonaceous chondrites (CC's), cometary dust particles, and ancient terrestrial rocks. These materials have been subject to considerable study, yet MMC formation pathways, metamorphic and alteration trends, and the means to clearly discern the origins of MMC types remain unclear. This symposium will explore how macromolecular carbon (MMC) evolves as a result of thermal, aqueous, radiolytic, and oxidative processing over time. We will highlight current state of the art technologies and the latest modeling efforts to characterize and study MMC, to constrain how organic molecules evolve into MMC, and to determine what signatures of their origins remain in matured materials.

General information about the conference can be found at: www.acs.org/meetings.
Any other inquiries should be directed to the symposium organizers:

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Interfacial Reactions under Nano-scale Confinement
Co-sponsored by ENVR, COLL

Confined water is abundant on the Earth, e.g., residing in nano-scale pores and grain boundaries of sedimentary rocks, interlayers of the clay minerals of shales, and nanometer thin films on mineral dust in the atmosphere. Despite the key importance of these nano-confined domains to energy generation, nuclear waste storage, and climate modeling, detailed fundamental explanations for the unique reactivity of confined aqueous solutions remain elusive and present a new and exciting frontier for geochemistry.

Nanoscale confinement fundamentally changes the chemical and physical properties of aqueous solutions, and this leads to surprising deviations in reactivity at the confined interfaces. Interfacial systems with confined water involve high solid-to-liquid ratios, overlapping electrical double layers from opposing surfaces, and additional interfaces terminated by other fluids or gasses. At a molecular scale, confined water is highly ordered and rotationally restricted by strong interactions with mineral surfaces, leading to relatively small dielectric permittivities and impacting solute mobilities. Because of these and other distinct properties of confined water, interfacial chemistry and reactivity under nano-scale confinement cannot be predicted based on known bulk-system thermodynamics and kinetics.

We invite contributions on mineral-water interfacial chemistry under confinement. A mechanistic and conceptual understanding of the key factors controlling reactivity in confined aqueous solutions requires an integrated approach, and both experimental, theoretical, and computational studies are encouraged. The topics to be covered in this session include, but are not limited to:

- properties of water under confinement
- influence of confinement on interface reactivity
- mass transport in nano-scale pores and water films
- nano-scale confinement effects on electron transfer
- confinement effects observed in field-scale studies
- dissolution, nucleation and growth under confinement
- impacts on thermodynamics and kinetics due to confinement
- novel experimental and computational methods for studying nanoconfined systems

General information about the conference can be found at: www.acs.org/meetings.
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Molecular Processes at Mineral-Water Interfaces

Mineral-water interfaces are ubiquitous in natural environments and prevalent in engineered and biological settings. Further, interfacial processes often exert controlling influences over mineral-containing systems. Though much understanding of interfacial processes has been achieved with the advent of high-resolution *in situ* techniques and computational methods, many significant questions and challenges remain.

This session highlights advances in experimental and computational methods that shape our current understanding of the mineral-water interface.

The topics to be covered in this session include, but are not limited to:

- New experimental/computational approaches in mineral-surface geochemistry
- Structure and reactivity of mineral surfaces
- Adsorption/desorption rates and mechanisms
- Surface mediated redox reactions
- Surface redox reactions of environmentally-relevant nanoparticles
- Interactions of environmental nanoparticles with contaminants and microorganisms

General information about the conference can be found at: www.acs.org/meetings.

Any other inquiries should be directed to the symposium organizers:

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Engineered Nanomaterials and Synthetic Macromolecules in the Environment: Fate, Behavior, and Effects

Advances in manufacturing and new applications have propelled the production and use of a wide variety of engineered nanomaterials (ENM), and synthetic macromolecules (SMM), in all aspects of life, from textiles to paints, from batteries to electronics, from building materials to medicine. The widespread adoption of these classes of materials stems from their unique properties compared to conventional materials that facilitate a number of desirable and beneficial effects, and they have become widely studied and increasingly well understood. On the other side of this spectrum, however, it is less certain how these materials behave once they enter the environment. ENM and SMM may be released into the environment at any point during the life-cycle of the ENM-/SMM-containing material, through handling, deterioration, accidental release or disposal. ENM and SMM may be more or less toxic than conventional materials, they may be more or less mobile, and they may be more or less persistent. What is the fate of these ENM and SMM? What is their behavior once they get there? What effects can they cause to environmental ecosystems? What is their bioavailability? Do they change chemically or morphologically, stabilize or deteriorate over time? Does it depend where or how they are released?

This second edition of the Symposium (first held in 2017 in Washington DC) aims to bring together experts who are addressing these uncertainties and developing the knowledge base for the safe use of ENM and SMM. We invite submissions that promote discoveries at the intersection of geochemistry, materials science, ecology and environmental sciences to address these and more questions. We seek submissions that look not only at understanding how currently-produced ENM and SMM behave in the environment (do they accumulate in sediment, remain suspended in water, or volatilize into the air), but also that are developing tools for predicting their behavior (e.g. fate descriptors) based on fundamental principles and material properties.

General information about the conference can be found at: www.acs.org/meetings.
Any other inquiries should be directed to the symposium organizers:

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Reactivity & Transformation of Manganese Oxides in Natural and Engineering Systems

Manganese (Mn) oxides are ubiquitous in natural environments, and actively involved in various biogeochemical processes that influence the fate and behaviors of metals, metalloids, organic compounds, as well as regulate the availability of nutrients. The unique properties of Mn oxides have also been utilized in a wide range of industrial applications in the fields of battery electrodes, catalysts, adsorbents, as well as semiconductors. This session invites contributions on Mn-oxide behavior in both natural and engineering systems that provide mechanistic understanding of the minerals' reactivity and phase transformation processes. This includes, but is not limited to topics such as: (biogenic) Mn oxides, adsorption, reduction, oxidation, dissolution, heterocatalysis, chemical reactors, fluid dynamics, kinetic experiments, real-time experiments, electron microscopic techniques and spectroscopic methods.

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Reactive Transport Modeling: A Cutting-Edge Tool for Investigating Coupled Processes

In natural and engineered systems, geochemical reactions (e.g. mineral dissolution-precipitation, redox reactions, sorption and radioactive decay) are intimately coupled with flow, transport, and heat exchange. The dynamic behavior of these systems is a result of the complex interplay between different processes. Reactive transport modeling, which solves simultaneously the conservation of mass, momentum and energy, provides a powerful tool to further our understanding of the contribution of individual factors and their compound effects. It has been widely applied to investigate processes and systems that are important in addressing our society's water and energy challenges, such as contaminant remediation in groundwater aquifers, CO₂ mineralization for carbon sequestration, or scaling in membrane systems. The development of mechanistic understanding of these coupled processes relies on continued refinement of the data and models that describe each process.

In this session, we invite contributions on recent advances in reactive transport modeling on topics that include but not limited to:

- improvement of thermodynamic and kinetic data
- integration of the electro-chemistry
- incorporation of nano-scale phenomena and molecular scale processes.

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