

Dear colleagues,

ACS Spring 2021 meeting is only one week away! We have lined up 10 exciting symposia with 158 oral and poster presentations.

Please see attached schedule for the Geochemistry Division program. The online scheduler is live at <https://www.acs.org/content/acs/en/meetings/acs-meetings.html>, where you can view all the ACS and GEOC events and technical programs.

All **oral presentations** will be live in Zoom. The **live poster session** is on **April 21<sup>st</sup> 9–10 am Pacific Time**. Each poster will be a breakout room in Zoom, where the presenter can deliver a poster or a 3-min lightening talk.

The Geochemistry Division will also hold a **virtual social hour** on **April 14<sup>th</sup> 12–1 pm Pacific Time**. You can access this from the virtual platform.

We look forward to seeing many of you!

Yuanzhi Tang  
Geochemistry Program Chair  
yuanzhi.tang@eas.gatech.edu



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



## Geochemistry Division Technical Program

Time zone: Pacific Daylight Time (US and Canada)

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

- 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
- 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

## GEOC Division Social Hour

Date: April 14<sup>th</sup>

Time: 12–1 pm Pacific Daylight Time (US and Canada)



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



## Congratulations to Spring 2021 Meeting Travel Award Recipients!

### Early Career Travel Award

Name	Affiliation	Abstract ID	Abstract title
Peng Yang	Argonne National Laboratory	3556361	Enhanced selenate uptake by lead co-sorption at the barite (001)–water interface
Qian Wang	Georgia Institute of Technology	3551409	Dynamic transformation of phosphorus and nitrogen during hydrothermal treatment (HT) of sewage sludge and resource recovery from HT process water
Xin Gu	Pennsylvania State University	3549795	Investigating weathering in shale across scales by tracking pseudomorphic transformation of pyrite
Youngjae Kim	Argonne National Laboratory	3550231	Replacement of Calcium Carbonate Polymorphs by Cerussite

### Student Travel Award

Name	Affiliation	Abstract ID	Abstract title
Bijoya Mandal	Temple University	3558361	Probing the interfacial solvent environment by measuring the vibrational lifetime of SCN <sup>-</sup> at the $\alpha$ -Al <sub>2</sub> O <sub>3</sub> (001)-aqueous interface
Andrew Freiburger	University of Victoria	3533908	A PHREEQC simulation of scaling during RO desalination
Ecenur Bulur	University of Wisconsin Madison	3555464	Transport-reaction modeling of particulate organic matter dynamics in riverbed sediments

**ACS Spring 2021 Schedule At a Glance**  
**(Geochemistry Program is highlighted in RED)**

**WEEK 1**

Pacific Time Zone (PDT)	Monday April 5	Tuesday April 6	Wednesday April 7	Thursday April 8	Friday April 9
7:00 AM – 8:00 AM	7-9:30 AM Opening Session				
8:00 AM – 9:00 AM			Keynote Event		Kavli Foundation Emerging Leader in Chemistry Lecture
9:00 AM – 12:00 PM	<b>GEOC 001A</b>	<b>GEOC 001C</b>	<b>GEOC 013B</b>	<b>GEOC 003A</b>	<b>GEOC 007A</b>
12:00 PM – 1:00 PM		GEOC 001 informal discussion	ACS SOCIAL HOUR		GEOC 007 informal discussion
1:00 PM – 4:00 PM	<b>GEOC 001B</b>	<b>GEOC 013A</b>	<b>GEOC 013C</b>	<b>GEOC 003B</b>	<b>GEOC 019A</b>
4:00 PM – 5:00 PM			GEOC 013 informal discussion	GEOC 003 informal discussion	GEOC 019 informal discussion
5:00 PM – 8:00 PM					Opening Reception 5-5:30 PM <b>Sci-Mix 5:30 – 8:00 PM</b>

<b>WEEK 2</b>					
Pacific Time Zone	Monday April 12	Tuesday April 13	Wednesday April 14	Thursday April 15	Friday April 16
7:00 AM – 8:00 AM					
8:00 AM – 9:00 AM	Fred Kavli Innovations in Chemistry Lecture		Keynote Event		Keynote Event
9:00 AM – 12:00 PM	<b>GEOC 011A</b>	<b>GEOC 011C</b> <b>GEOC 005A</b>	<b>GEOC 005C</b> <b>GEOC 021A</b>	<b>GEOC 017A</b>	<b>GEOC 015A</b>
12:00 PM – 1:00 PM		ACS SOCIAL HOUR	<b>GEOC social event</b>	ACS SOCIAL HOUR	GEOC 015 informal discussion
1:00 PM – 4:00 PM	<b>GEOC 011B</b>	<b>GEOC 011D</b> <b>GEOC 005B</b>	<b>GEOC 005D</b>	<b>GEOC 017B</b>	
4:00 PM – 5:00 PM		GEOC 011 informal discussion	GEOC 005 informal discussion	GEOC 017 informal discussion	

<b>WEEK 3</b>					
	Monday April 19	Tuesday April 20	Wednesday April 21	Thursday April 22	Friday April 23
9:00 AM – 10:00 AM			<b>Live Poster Session</b>		
24hr	On Demand Technical Sessions	On Demand Technical Sessions	On Demand Technical Sessions	On Demand Technical Sessions	On Demand Technical Sessions

<b>WEEK 4</b>					
	Monday April 26	Tuesday April 27	Wednesday April 28	Thursday April 29	Friday April 30
24hr	On Demand Technical Sessions	On Demand Technical Sessions	On Demand Technical Sessions	On Demand Technical Sessions	On Demand Technical Sessions

## ACS Spring 2021 Geochemistry Program - Oral Presentations

Date	Session	Presentation Time		Abstract ID	First Name	Last Name	Abstract Title
<b>Monday</b> <b>04/05/2021</b>	40 Years of High-Resolution NMR Spectroscopy of Inorganic Solids	9:00 AM	9:10 AM				Introductory Remarks
		9:10 AM	9:35 AM	3555183	Karl	Mueller	Solids, surfaces, computers, and pencils: Targets and tools for solid-state NMR
		9:35 AM	10:00 AM	3533519	Mark E	Smith	<sup>29</sup> Si and <sup>27</sup> Al magic angle spinning NMR of oxynitride ceramics
		10:00 AM	10:25 AM	3541747	Ian	Farnan	High-resolution nuclear magnetic resonance of highly radioactive solids: strategies and applications in radiation damage
		10:25 AM	10:35 AM				Intermission
		10:35 AM	11:00 AM	3543181	Danielle	Laurencin	Unraveling the structure and reactivity of interfacial oxygen sites thanks to oxygen-17 mechanochemical labeling and high resolution NMR
		11:00 AM	11:15 AM	3553504	Chia-Hsin	Chen	<sup>17</sup> O isotopic labeling of silica and titania using mechanochemistry: an investigation of enrichment mechanisms
		11:15 AM	11:30 AM	3549390	Ieva	Goldberga	Oxygen-17 isotopic enrichment of calcium oxalate monohydrate phase
<b>Monday</b> <b>04/05/2021</b>	40 Years of High-Resolution NMR Spectroscopy of Inorganic Solids	1:00 PM	1:05 PM				Introductory Remarks
		1:05 PM	1:30 PM	3558239	Eric	Walter	In Situ Investigations of geochemical, extremophile and catalytic systems by high pressure: high temperature MAS-NMR
		1:30 PM	1:45 PM	3529747	Geoffrey	Bowers	Linking NMR spectroscopy and computational molecular modeling to understand layer structure material
		1:45 PM	2:10 PM	3558165	Sophia	Hayes	<sup>29</sup> Si chemical shift tensors: From NMR experiments to computational prediction
		2:10 PM	2:20 PM				Intermission
		2:20 PM	2:45 PM	3555785	Jorgen	Skibsted	<sup>29</sup> Si and <sup>27</sup> Al MAS NMR studies of Portland cements and zeolites
		2:45 PM	3:10 PM	3552222	Mattias	Eden	Solid state NMR and molecular dynamics simulation studies of phosphoserine-doped calcium phosphate cements with bone-adhesive properties
		3:10 PM	3:35 PM	3533614	christian	bonhomme	Hydroxyapatite revisited by DNP and spin diffusion: Natural abundance <sup>43</sup> Ca DNP MAS and ultra high magnetic field (35T) <sup>43</sup> Ca experiments, modeling and new mathematical treatment of dynamic nuclear polarization processes
<b>Tuesday</b> <b>04/06/2021</b>	40 Years of High-Resolution NMR Spectroscopy of Inorganic Solids	9:00 AM	9:05 AM				Introductory Remarks
		9:05 AM	9:30 AM	3553588	Pierre	Florian	Getting the most information from the worst resolution: NMR of disordered solids
		9:30 AM	9:45 AM	3553571	Cesar	Leroy	In-depth atomic-scale structure and surface acidity description of aluminum oxide layers by ssNMR and DNP SENS spectroscopies
		9:45 AM	10:10 AM	3552195	Randall	Youngman	Enabling glass-ceramic research with NMR
		10:10 AM	10:20 AM				Intermission
		10:20 AM	10:45 AM	3553824	Hellmut	Eckert	The glassy part of glass ceramics: Structural insights from solid state NMR
		10:45 AM	11:00 AM	3554512	Brian	Phillips	Insights from NMR spectroscopy on the diversity of boron defects in calcite
		11:00 AM	11:25 AM	3548610	Yining	Huang	High-resolution SSNMR: Insights into the structure and chemistry of metal-organic frameworks
		11:25 AM	11:50 AM	3556193	philip	grandinetti	Statistical learning of NMR tensors from 2D Si-29 isotropic/anisotropic correlation nuclear magnetic resonance spectra of silicate glasses
<b>Tuesday</b> <b>04/06/2021</b>	Molecular Processes at Mineral-Water Interfaces	1:00 PM	1:05 PM				Introductory Remarks
		1:05 PM	1:35 PM	3552508	Marie	Gaigeot	Silica-water interfaces as a good platform/playfield for revealing hydrophilic to hydrophobic structural order of interfacial water
		1:35 PM	2:00 PM	3555031	Jing	Zhang	Multi-technique approach on the adsorption of mono- and poly-vanadate (V(V)Q <sup>3-</sup> ) onto hematite

		2:00 PM	2:30 PM	3551295	Sang Soo	Lee	Salinity dependent evolution of the electrical double layer at the muscovite (001) water interface
		2:30 PM	2:40 PM				Intermission
		2:40 PM	3:10 PM	3557830	Ian	Bourg	Dielectric spectra of water in charged clay interlayer nanopores
		3:10 PM	3:35 PM	3552556	Somaiyeh	Dadashi	Influence of the spatially heterogeneous charge distribution on Al <sub>2</sub> O <sub>3</sub> (0001) on the interfacial organization of acetonitrile-water mixtures
		3:35 PM	4:00 PM	3558361	Bijoya	Mandal	Probing the interfacial solvent environment by measuring the vibrational lifetime of SCN <sup>-</sup> at the Al <sub>2</sub> O <sub>3</sub> (0001)-aqueous interface
<b>Wednesday</b>	<b>GEOC013B</b>	9:00 AM	9:30 AM	3554306	Susan	Rempe	Differentiating aqueous halide ions, locally: F, Cl, Br, I
<b>04/07/2021</b>	Molecular Processes	9:30 AM	9:55 AM	3554810	Jacquelyn	Bracco	Cation sorption at the barite (001)- and (210)-water interfaces
	at Mineral-Water	9:55 AM	10:15 AM	3552905	Inva	Braha	Pb desorption at the barite (001)-water interface
	Interfaces	10:15 AM	10:20 AM				Intermission
		10:20 AM	10:50 AM	3558578	John	Bargar	Importance of organic matter as a control over U(IV)- and Pb(II)-surface interactions in natural sediments
		10:50 AM	11:15 AM	3554139	Evert	Elzinga	Trace metal sorption by green rust: Macroscopic and spectroscopic analyses
		11:15 AM	11:40 AM	3551067	Elizabeth	Tomaszewski	Organic matter adsorption and fractionation to ferrihydrite under different salinity conditions
		11:40 AM	12:00 PM	3538141	Alon	Rabinovich	Effect of phenolic organics on struvite precipitation from simulated dairy wastewater
<b>Wednesday</b>	<b>GEOC013C</b>	1:00 PM	1:30 PM	3554907	Sebastien	Kerisit	Molecular-scale controls on heterogeneous nucleation and growth at mineral-water interfaces
<b>04/07/2021</b>	Molecular Processes	1:30 PM	1:55 PM	3556361	Peng	Yang	Enhanced selenate uptake by lead co-sorption at the barite (001)-water interface
	at Mineral-Water	1:55 PM	2:20 PM	3544912	Ruiyu	Wang	On the role of Alumina in the origin of life: Surface driven assembly of amino acids
	Interfaces	2:20 PM	2:30 PM				Intermission
		2:30 PM	3:00 PM	3551643	Alicia	Schuitemaker	Atomic structure and dynamics at the calcium carbonate (CaCO <sub>3</sub> ) vaterite water interface
		3:00 PM	3:25 PM	3555109	Anshuman	Satpathy	U(VI) reduction by structural iron(II) present in montmorillonite
		3:25 PM	3:50 PM	3557923	Logan	Augustine	DFT + thermodynamics method to study inner-sphere adsorption occurring at the mineral-water interface
		3:50 PM	3:55 PM				Concluding Remarks
<b>Thursday</b>	<b>GEOC003A</b>	9:00 AM	9:05 AM				Introductory Remarks
<b>04/08/2021</b>	Fundamental	9:05 AM	9:25 AM	3551260	Paul	Fenter	Understanding extrinsic controls to mineral water interfacial reactivity
	Reactions Driving	9:25 AM	9:45 AM	3552810	Alejandro	Fernandez-Martinez	Probing the structure and reactivity of iron and aluminum minerals towards rare earth elements in acid mine drainage
	Macroscopic						
	Geochemical	9:45 AM	10:05 AM	3548553	Eric	Ferrage	Upscaling strategies for the analysis of water diffusion in clay porous media
	Processes	10:05 AM	10:25 AM	3557786	David	Cole	Nanopore confinement of C-H-O mixed-volatile fluids relevant to subsurface energy systems
		10:25 AM	10:35 AM				Intermission
		10:35 AM	10:55 AM	3559051	Alexis	Navarre-Sitchler	Connecting the dots between fluid transport, physical heterogeneity, and the lab-field dissolution rate discrepancy
		10:55 AM	11:15 AM	3534018	Anthony	Ladd	Evolution of grain shapes by dissolution: Validation and upscaling of pore-scale simulations
		11:15 AM	11:35 AM	3557372	Hang	Deng	Multi-scale investigation of the dynamic evolution of mineral coating
		11:35 AM	11:55 AM	3549795	Xin	Gu	Investigating weathering in shale across scales by tracking pseudomorphic transformation of pyrite
<b>Thursday</b>	<b>GEOC003B</b>	1:00 PM	1:05 PM				Introductory Remarks

<b>04/08/2021</b>	Fundamental Reactions Driving Macroscopic Geochemical Processes	1:05 PM	1:25 PM	3535579	James	Kubicki	Density functional theory modeling of Ba <sup>2+</sup> and SO <sub>4</sub> <sup>2-</sup> adsorption onto the quartz (101) surface
		1:25 PM	1:45 PM	3558334	Lawrence	Anovitz	Frustrated coulombic and cation size effects on boehmite aggregation: a tumbler small- and ultra-small angle neutron scattering study
		1:45 PM	2:05 PM	3552170	Li	Li	From pores to watersheds: reactions at interfaces
		2:05 PM	2:25 PM	3554240	Narasimhan	Loganathan	Interaction of natural organic matter with smectite mineral surfaces: A combined experimental and simulation study
		2:25 PM	2:35 PM				Intermission
		2:35 PM	2:55 PM	3529936	Emily Wei-Hsin	Sun	Molecular dynamics simulations of water thin films, contact angles, and capillary pressure in a quartz nanopore in the presence of CO <sub>2</sub> and organic molecules
		2:55 PM	3:15 PM	3533743	Juliane	Weber	The influence of microstructure on mineral dissolution-precipitation: The model systems of CaCO <sub>3</sub> -CaMg(CO <sub>3</sub> ) <sub>2</sub> and CaCO <sub>3</sub> -FeCO <sub>3</sub>
		3:15 PM	3:35 PM	3550231	YoungJae	Kim	Replacement of calcium carbonate polymorphs by cerussite
		3:35 PM	3:45 PM				Concluding Remarks

<b>Friday</b>	<b>GEOC007A</b>	9:00 AM	9:05 AM				Introductory Remarks
<b>04/09/2021</b>	Biogeochemical Transformation in the Underground Environment – Natural Processes and Engineered Implementations for Contaminant Abatement	9:05 AM	9:30 AM	3562474	Matthew	Ginder-Vogel	Impact of dissolved organic matter on phenolic contaminant oxidation by manganese oxides
		9:30 AM	9:55 AM	3529909	Matthew	Berens	Assessment of 2,4-Dinitroanisole transformation using compound specific isotope analysis after in situ chemical reduction of iron oxides
		9:55 AM	10:10 AM	3557554	Kevin	Hickey	Modeling the reduction of nitroaromatics and munition constituents by humic acid using quantum chemically computed reaction energies and quinone-like functional groups
		10:10 AM	10:25 AM	3555511	Arata	Katayama	Alternate functionality of humin, a solid-phase humic substance, as extracellular electron mediator in carbon dioxide-reducing acetogenesis
		10:25 AM	10:35 AM				Intermission
		10:35 AM	10:50 AM	3544059	Merritt	Logan	Ultrahigh resolution mass spectrometry analysis of organic nitrogen released upon permafrost thaw
		10:50 AM	11:05 AM	3551900	Holly	Roth	Impact of beaver ponds on biogeochemical cycling of organic nitrogen within a fire-impacted watershed
		11:05 AM	11:20 AM	3530563	William	Bahureksa	Wildfire severity impacts on chemical transformation of soil organic carbon and nitrogen
		11:20 AM	11:35 AM	3555525	Samantha	Fuchs	Geochemical and geomechanical alteration by acidic brine of artificially fractured sandstone under strain
		11:35 AM	11:50 AM	3549586	Maedeh	Soleimanifar	Utilization of cerium oxide and neodymium oxide nanoparticles by Methylobacterium extorquens (ATCC 14718)
		11:50 AM	11:55 AM				Concluding Remarks

<b>Friday</b>	<b>GEOC019A</b>	1:00 PM	1:05 PM				Introductory Remarks
<b>04/09/2021</b>	Reactive Transport Modeling: A Cutting-Edge Tool for Investigating Coupled Processes	1:05 PM	1:25 PM	3557733	Young-Shin	Jun	Reactive transport modeling to decipher dissolution and nucleation at the interface of supercritical CO <sub>2</sub> -brine-cement
		1:25 PM	1:40 PM	3557748	Sergi	Molins	Expanding the role of pore-scale reactive transport models to capture the multiscale evolution of fractured media
		1:40 PM	1:55 PM	3555749	Qian	Zhang	Investigation of reactive transport processes in a fractured dolostone via multi-scale simulations
		1:55 PM	2:15 PM	3553922	Lauren	Beckingham	Improving understanding of mineral reaction rates and permeability evolution in porous media

		2:15 PM	2:30 PM	3549763	Olubukola	Ishola	Application of machine learning to predict hydraulic tortuosity of highly heterogeneous porous media
		2:30 PM	2:35 PM				Intermission
		2:35 PM	2:50 PM	3557280	Vitalii	Starchenko	Mineral precipitation in porous media: Quantification of X-ray tomography data and pore-scale reactive transport simulations
		2:50 PM	3:05 PM	3548753	Adedapo	Awolayo	Investigation of accessible reactive surface area for improved prediction of CO <sub>2</sub> mineralization in basaltic aquifer rocks
		3:05 PM	3:25 PM	3558549	Hang	Wen	Climatic controls on organic carbon transformation and transport at the hillslope scale
		3:25 PM	3:45 PM	3533908	andrew	freiburger	A PHREEQC simulation of scaling during RO desalination
		3:45 PM	4:00 PM	3554271	Mengnan	Li	Higher-order finite element multiphase reactive transport model for unstructured and fractured grids: benchmark studies, scaling analysis, and applications to CO <sub>2</sub> sequestration

<b>Monday</b>	<b>GEOC011A</b>	9:00 AM	9:05 AM				Introductory Remarks
<b>04/12/2021</b>	Interfacial Reactions under Nano-scale Confinement	9:05 AM	9:35 AM	3539187	Sophie	LE CAER	Confined water in aluminosilicate nanotubes: Structure, dynamics and the importance of charge separation effects upon irradiation
		9:35 AM	10:05 AM	3551840	Sylvie	Roke	The interfacial structure of water under confinement
		10:05 AM	10:35 AM	3557408	Ian	Bourg	Coupled fluxes of water and ions (NaCl) during flow through silica nanopores
		10:35 AM	10:50 AM				Intermission
		10:50 AM	11:10 AM	3555209	Yaguang	Zhu	Solution pH in nanopores is controlled by ionic surface propensities
		11:10 AM	11:40 AM	3557092	Ward	Thompson	Dynamics and spectroscopy of liquids in nanoscale amorphous silica pores

<b>Monday</b>	<b>GEOC011B</b>	1:00 PM	2:00 PM	3534972	Vicki	Grassian	Interfacial reactions involving thin films of particles
<b>04/12/2021</b>	Interfacial Reactions under Nano-scale Confinement	2:00 PM	2:30 PM	3556885	Sebastien	Kerisit	Diffusion controls on divalent metal silicate carbonation in confined water films
		2:30 PM	2:40 PM				Intermission
		2:40 PM	3:10 PM	3558407	Ke	Yuan	Understanding the nucleation and growth of barite by optical microscopy and X-ray nanotomography
		3:10 PM	3:30 PM	3558138	John	Loring	Low temperature magnesite growth during forsterite carbonation in thin H <sub>2</sub> O films
		3:30 PM	4:00 PM	3557633	David	Cole	Probing the olivine-water interface: Experimental and molecular simulation perspectives

<b>Tuesday</b>	<b>GEOC005A</b>	9:00 AM	9:20 AM	3556912	Katherine	Hull	Insights on shale iron leaching and secondary mineral crystallization through phase and morphology analysis
<b>04/13/2021</b>	Crystallization Pathways: New Perspectives on Nucleation, Growth & Dissolution of Natural & Synthetic Materials	9:20 AM	9:40 AM	3548893	MARIA	MEZA	Determination of solubility constants and thermodynamic variables for uranyl arsenate solids containing monovalent cations sodium (Na) and potassium (K)
		9:40 AM	10:10 AM	3558347	Ian	Bourg	Adsorption and aggregation of soil organic matter at the clay-water interface
		10:10 AM	10:20 AM				Intermission
		10:20 AM	10:50 AM	3561945	Bart	Kahr	Helicoidal Growth and Charge Transport
		10:50 AM	11:10 AM	3557445	Maria	Sushko	Role of interfacial structure and dynamics in driving non-classical crystallization
		11:10 AM	11:30 AM	3548885	Tyler	Schmidt	Metadynamics simulations of ion detachment from calcite (104)
		11:30 AM	12:00 PM	3556170	Kristen	Fichthorn	Kinetics of halide-mediated Cu nanowire growth

<b>Tuesday</b>	<b>GEOC011C</b>	9:00 AM	9:30 AM	3561280	Laura	Fumagalli	Direct measurement of the anomalously low dielectric constant of confined water
<b>04/13/2021</b>	Interfacial Reactions under Nano-scale Confinement	9:30 AM	10:00 AM	3562541	Derk	Joester	Crystallization Kinetics of Amorphous Carbonates in Confinement
		10:00 AM	10:30 AM	3532462	Young-Shin	Jun	Calcium phosphate's nucleation kinetics and energy barrier in nanoscale confined organic spaces
		10:30 AM	10:45 AM				Intermission



		10:45 AM	11:05 AM	3537502	Kevin	Leung	Interplay of physically different properties leading to challenges in separating lanthanide cations -- an Ab Initio molecular dynamics and experimental study
		11:05 AM	11:35 AM	3530552	Tina	Nenoff	In situ PDF/DRIFTS Study of the role of water in Ag particle formation in zeolites
		11:35 AM	11:55 AM	3552217	Anastasia	Ilgen	Adsorption of lanthanides at nanoconfined silica and alumina-water interfaces
<b>Tuesday</b> <b>04/13/2021</b>	<b>GEOC005B</b> Crystallization	1:00 PM	1:30 PM	3557764	R Lee	Penn	Formation, growth, dissolution, and transformation of nanoparticles in reactive liquid media
	Pathways: New	1:30 PM	1:50 PM	3537710	Guomin	Zhu	Self-similar mesocrystals form via interface-driven nucleation and assembly
	Perspectives on	1:50 PM	2:10 PM	3542434	Michel	Sassi	Structure and composition of ferrihydrite nanoparticles from Ab Initio thermodynamics
	Nucleation, Growth						Intermission
	& Dissolution of	2:10 PM	2:25 PM				
	Natural & Synthetic	2:25 PM	2:45 PM	3550362	Alireza	Namayandeh	System chemistries control the formation and transformation kinetics of Fe <sub>3</sub> like clusters
	Materials	2:45 PM	3:05 PM	3555429	Si	Chen	Observation and synthesis of exceptionally Fe-deficient "hydrohematite" and "hydrogoethite"
		3:05 PM	3:35 PM	3557791	Young-Shin	Jun	Nucleation kinetics and thermodynamics of iron(III) (hydr)oxide nanoparticles forming on quartz
<b>Tuesday</b> <b>04/13/2021</b>	<b>GEOC011D</b> Interfacial Reactions	1:00 PM	1:20 PM	3553974	Jeffery	Greathouse	Synergistic effects of nanoconfinement and surface charge on iron adsorption on mesoporous silica
	under Nano-scale	1:20 PM	1:50 PM	3561911	Michael	Whittaker	Dynamic clay microstructures emerge via ion complexation waves at the mineral interface
	Confinement						
<b>Wednesday</b> <b>04/14/2021</b>	<b>GEOC005C</b> Crystallization	9:00 AM	9:30 AM	3555661	Xin	Zhang	Unravel particle-mediated crystallization pathways via using advanced transmission electron microscopy techniques
	Pathways: New	9:30 AM	10:00 AM	3556987	Qian	Chen	In-situ TEM based cinematography to elucidate crystallization pathways at the nanoscale
	Perspectives on						Intermission
	Nucleation, Growth	10:00 AM	10:15 AM				
	& Dissolution of	10:15 AM	10:45 AM	3554328	F. Marc	Michel	Impacts of initial Ca/P on the formation and transformation of amorphous calcium phosphate
	Natural & Synthetic						
	Materials	10:45 AM	11:05 AM	3543217	Rogier	Besselink	High energy X-ray Scattering revealing the short-range order of a metastable proto-CSH phase and its implications on cement nucleation
		11:05 AM	11:25 AM	3555401	Yarong	Qi	Role of organic foulants on the kinetics of silica scaling: Behavior and mechanisms
		11:25 AM	11:45 AM	3555710	Andrew	Lauer	Multi-step nucleation in strontium sulfate: Reaction mechanisms and a hemihydrated precursor
<b>Wednesday</b> <b>04/14/2021</b>	<b>GEOC021A</b> General	9:00 AM	9:25 AM	3551409	Qian	Wang	Dynamic transformation of phosphorus and nitrogen during hydrothermal treatment (HT) of sewage sludge and resource recovery from HT process water
	Geochemistry	9:25 AM	9:45 AM	3551347	Chelsea	Neil	Effects of water saturation on noble gas diffusion through zeolitic tuff
		9:45 AM	10:05 AM	3554066	Hasini	Senanayake	Simulations of the IR and raman spectra of water confined in amorphous silica slit pores
		10:05 AM	10:20 AM				Intermission
		10:20 AM	10:40 AM	3556958	Hidemitsu	Katsura	The variation of air radiation dose rates from December 2019 to March 2020 inside cabin flights between Tokyo and Singapore or Tokyo and Kuala Lumpur
		10:40 AM	11:00 AM	3549462	Yunpo	Li	Geochemical indicators in northeastern Pennsylvania groundwater are consistent with natural methane sources
		11:00 AM	11:20 AM	3551837	Florence	Ling	Modeling CaSiO <sub>3</sub> -CO <sub>2</sub> reactions and permeability evolution for sealing leakages from geologic carbon storage
<b>Wednesday</b>	<b>GEOC005D</b>	1:00 PM	1:30 PM	3562543	Jeffrey	Rimer	Crystallization in Reverse: Tailoring the Cooperative Action of Demineralizing Agents

<b>04/14/2021</b>	Crystallization	1:30 PM	1:50 PM	3555229	Yaguang	Zhu	Roles of sulfate in the nucleation, growth, and Ostwald ripening of CaCO <sub>3</sub> on quartz
	Pathways: New Perspectives on	1:50 PM	2:10 PM	3557707	Sebastian	Mergelsberg	Nucleation of mixed-cation amorphous carbonate precursors: Example of cadmium in ACC and vaterite
	Nucleation, Growth & Dissolution of	2:10 PM	2:25 PM	3533650	christian	bonhomme	Intermission
	Natural & Synthetic Materials	2:25 PM	2:45 PM				In situ description of biomineralization processes and pre-crystalline phases studied by solid state NMR: The study case of hydrated calcium oxalates
		2:45 PM	3:15 PM	3553298	Juan Diego	Rodriguez-Blanco	New insights into the mechanisms of bastn�site formation
<b>Thursday</b>	<b>GEOC017A</b>	9:00 AM	9:05 AM				Introductory Remarks
<b>04/15/2021</b>	Reactivity & Transformation of	9:05 AM	9:25 AM	3550224	Jeffrey	Post	Raman spectroscopy identification and characterization of natural and synthetic manganese oxides
	Manganese Oxides in Natural and	9:25 AM	9:45 AM	3554532	Zhenwei	Gao	Photochemically-induced co-oxidation of Mn <sup>2+</sup> and Co <sup>2+</sup> and the formation of Co <sup>III</sup> -incorporated Mn <sup>IV</sup> oxides
	Engineering Systems	9:45 AM	10:05 AM	3557692	Young-Shin	Jun	Effects of reactive halogen species on the formation of photochemically-induced abiotic Mn <sup>IV</sup> oxides
		10:05 AM	10:25 AM	3553890	Daniel	Strongin	Redox chemistry and structural transformations relevant to birnessite as an electrocatalyst for water oxidation
		10:25 AM	10:40 AM				Intermission
		10:40 AM	11:00 AM	3529807	James	Kubicki	Macroscopic and molecular understanding of Np(V) sorption on the birnessite-water interface
		11:00 AM	11:20 AM	3557644	Martial	Taillefert	Insights into the mechanism of reduction of manganese oxides by thiols and arsenite
	11:20 AM	11:40 AM	3538820	Boyoung	Song	Transmission electron microscopy (TEM) investigation of aggregate structures and their impacts on reactivity of manganese oxide mixtures	
		11:40 AM	12:00 PM	3555499	Matthew	Fischel	Kinetics of arsenic oxidation by naturally formed manganese-oxides
<b>Thursday</b>	<b>GEOC017B</b>	1:00 PM	1:20 PM	3554994	Yuanzhi	Tang	Redox cycling driven transformation of layered manganese oxides to tunnel structures
<b>04/15/2021</b>	Reactivity & Transformation of	1:20 PM	1:40 PM	3556564	Mengqiang	Zhu	Mn(II)-promoted phase transformation of manganese oxides
	Manganese Oxides in Natural and	1:40 PM	2:00 PM	3557603	Peng	Yang	Mn(II)-driven redox transformation of layered Mn oxides in seawater
	Engineering Systems	2:00 PM	2:20 PM	3553589	Seonyi	Namgung	Adsorbed Mn(II) formed Mn oxide nano-needles on the tip of goethite particles when exposed to oxygen
		2:20 PM	2:25 PM				Intermission
		2:25 PM	2:45 PM	3558300	Jasquelin	Pena	The fate of bioavailable carbon sources in presence of manganese oxides
		2:45 PM	3:05 PM	3557589	Margaret	Hinkle	Trace metal uptake by biogenic manganese oxides with structural variability: Connecting lessons from coal mine drainage remediation and the laboratory
		3:05 PM	3:25 PM	3556732	Michael	Zdilla	Experimental optimization of layered manganese oxide water-oxidation catalysts by nano-level organizational control guided by molecular dynamics and quantum calculation
		3:25 PM	3:45 PM	3530184	Amritpal Singh	Chaddha	Rock varnish: Potential future product
<b>Friday</b>	<b>GEOC015A</b>	9:00 AM	9:10 AM				Introductory Remarks
<b>04/16/2021</b>	Engineered Nanomaterials and	9:10 AM	9:40 AM	3556469	Eduardo	Rodrigues	Uptake and accumulation of cerium oxide nanoparticles, as environmental contaminants, by soybean plants
	Synthetic Macromolecules in	9:40 AM	10:10 AM	3556469	Rafael	Santos	Photodegradation of Quantum Dots: A New Kinetic Model and Significance of Structural Parameters
	the Environment: Fate, Behavior, and	10:10 AM	10:20 AM	3558661	Pooya	Paydary	Concluding Remarks

**ACS Spring 2021 Geochemistry Program - Poster Presentations**  
**April 21 (Wednesday) 9 - 10 am Pacific Time**

Session	Symposia Title	Abstract ID	First Name	Last Name	Abstract Title
GEOC004A	Fundamental Reactions Driving Macroscopic Geochemical Processes	3554218	Matthew	Siebecker	Experimental redox kinetics of nanoparticulate manganese oxide (MnO <sub>2</sub> ) and dissolved organic carbon: UV-Vis study
		3551878	Erin	Berns	Proton: Binding model to simulate pH buffering in Arctic tundra soils
GEOC006A	Crystallization Pathways: New Perspectives on Nucleation, Growth & Dissolution of Natural & Synthetic Materials	3534016	Connor	Schmidt	Mesoscale structure of Ediacaran and synthetic dolomite spherulites
		3552291	Yi	Ren	Effects of pH on immersion freezing by kaolinite
		3554264	Michela	La Bella	Diffraction: tomography investigations on the hydration of gypsum plaster
GEOC008A	Biogeochemical Transformation in the Underground Environment – Natural Processes and Engineered Implementations for Contaminant Abatement	3557425	Danhui	Xin	Comparison of mediated electrochemical analysis and chemical redox titration for measuring the electron storage capacity of biochar
GEOC014A	Molecular Processes at Mineral-Water Interfaces	3530557	Anand	Kumar	Aqueous alteration of potassium-rich feldspar and effects on its ice nucleation ability
		3550878	Alicia	Moya	Carbonate rocks reactivity across scales: elucidating the role of biominerals
		3552375	Abhishek	Soni	Heterogeneous ice nucleation on the muscovite mica surface
		3556315	Anita	Sanchez	Sorption of methylated arsenic onto mackinawite (FeS)
		3546517	Ruiyu	Wang	Water hydrophilic behavior at aqueous/alumina interfaces
GEOC018A	Reactivity & Transformation of Manganese Oxides in Natural and Engineering Systems	3549750	Edwin	Rivas Meraz	Remediation of mercury: Contaminated aquatic sediments with manganese(IV) oxide and activated carbon amendments
GEOC020A	Reactive Transport Modeling: A Cutting-Edge Tool for Investigating Coupled Processes	3555464	Ecenur	Bulur	Transport-reaction modeling of particulate organic matter dynamics in riverbed sediments
GEOC022A	General Geochemistry	3550428	Samantha	James	HF: Free extraction technique of particulate organic matter from sedimentary rocks
		3553236	Boris	Lau	Temperature effects on the interactions of soil organic matter with hematite and goethite: Perspectives on bulk and nano-scale sorption
		3554628	Amelia	Bunnell	Sample preconcentration and matrix removal via SPE for the determination of dissolved hydrolyzable amino acids in estuarine samples via liquid chromatography tandem mass spectrometry
		3557468	Reza	Khalidy	Geochemical modeling applications and research hot spots - a scientometric and critical review of 2019
		3557738	Alejandro	Briso	A simple geochemical approach to identify scenarios for managing drinking water treatment residuals (DWTRs)
		3558422	Tiara	Ogus	Phosphorus cycling and retention in agriculturally dominated stream ecosystems in semi-arid Mediterranean climates



2021 ACS Fall National Meeting  
August 22-26, 2021, Atlanta, GA  
*Resilience of Chemistry*



<https://communities.acs.org/t5/Geochemistry-Division/gh-p/geoc-division>

## Geochemistry Division

### Call for Abstract Submission

Abstract submission: March 15, 2021 – April 12, 2021

Meeting time: August 22 – 26, 2021

Meeting format: Both in-person and 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\*:

- Symposium in Honor of Prof. Michael Hochella, 2021 Geochemistry Medal Recipient
- Interfaces for Society: The Next Frontier
- Experimental and computational approaches to molecular-scale understanding of mineral-fluid interactions (Session in memory of R. James Kirkpatrick)
- The Evolution of Macromolecular Carbon through Space and Time
- Advances in Ultrahigh Resolution Mass Spectrometry for Tracking Natural Organic Matter in Global Systems
- Experimental and Modelling Approaches for Nucleation in Porous Media
- Molecular scale processes of phosphorus cycling in natural and engineered systems
- Undergraduate Research in Geochemistry
- General Geochemistry

\*organizer contact information and symposium descriptions are attached.

**Abstract submission:** Please submit your abstracts using the ACS Meeting Abstracts Programming System (MAPS) at <http://maps.acs.org>. The abstract submission window is March 15, 2021 – April 12, 2021.

### Questions?

- For questions about specific symposia, please contact the organizers directly.
- For general questions about the Geochemistry Division symposia and activities, please contact Adam Wallace ([afw@udel.edu](mailto:afw@udel.edu)).



2021 ACS Fall National Meeting  
August 22-26, 2021  
Atlanta, GA  
*Resilience of Chemistry*



## Geochemistry Division

### Call for Travel Award application (Due date: April 12, 2021)

Dear colleagues,

We are pleased to applications for the Geochemistry Division's **Student Travel Award** and **Early Career Scientist Travel Award** for the Fall 2021 ACS National Meeting to be held August 22–26, 2021 in Atlanta, GA. Note that the meeting format is currently scheduled as hybrid (both in-person and virtual) and that the registration rates are not yet set. See below for award descriptions and procedures.

#### Student Travel Award

- **Number of awards:** Up to 8 awards based on the quality of the applications.
- **Award:** (1) The Geochemistry Division will pay for the awardees' registration for the ACS National Meeting at the corresponding ACS member rate. (2) Awardees will be given an extended time allocation (typically 25-30 minutes) for their oral presentations.
- **Eligibility:** (1) The applicant must be an undergraduate or graduate student. (2) The applicant must have already submitted a regular abstract to MAPS for the meeting (see Application Procedure for details). (3) The applicant must be the presenting author. (4) Only one application per presenting author will be considered.

#### Early Career Scientist Travel Award

- **Number of awards:** Up to 2 awards based on the quality of the applications.
- **Award:** (1) The Geochemistry Division will pay for the awardees' registration for the ACS National Meeting at the corresponding ACS member rate. (2) Awardees will be given an extended time allocation (typically 25-30 minutes) for the oral presentation.
- **Eligibility:** (1) The applicant must have received their PhD degree within 5 years of the abstract submission deadline (April 12, 2021). (2) The applicant must have already submitted a regular abstract to MAPS for the meeting (see Application Procedure for details). (3) The applicant must be the presenting author. (4) Only one application per presenting author will be considered.

#### Application Procedures

- Submitting your regular abstract to the ACS Meeting Abstract Programming System (MAPS <http://maps.acs.org>) before the due date (April 12, 2021).
- Submit a separate, extended abstract to the GEOC Program Chair at: [afw@udel.edu](mailto:afw@udel.edu)
- Extended abstracts should not exceed one page (use at least 11-pt font, single-line spacing, and 1-inch margins) and may contain tables and figures (counted toward the page limit). Make sure to (1) include your name, affiliation, abstract title, and abstract number, and (2) indicate whether you are an undergraduate/graduate student (for the Student Travel Award) or your PhD degree date/year (for the Early Career Scientist Travel Award).
- Applications must be received during the abstract submission window (March 15, 2021–April 12, 2021).



2021 ACS Fall National Meeting  
August 22-26, 2021  
Atlanta, GA  
*Resilience of Chemistry*



### Evaluation

- Abstracts will be judged based on the impact on the field of geochemistry, technical approach, quality and clarity of writing, relevance of the abstract to the symposia and national meeting themes, and balance among different symposia.
- Award winners will be announced by the end of May, 2021.

### Questions?

- General information about the conference can be found at:  
<https://www.acs.org/content/acs/en/meetings/national-meeting.html>
- Questions about the awards should be directed to [afw@udel.edu](mailto:afw@udel.edu)