

## IAN C BOURG

Civil & Environmental Engineering / Princeton Environmental Institute  
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### EDUCATION

PhD, Civil and Environmental Engineering, University of California, Berkeley (2004).  
Advisor: G Sposito  
MSc, Chemical Engineering, National Institute of Applied Sciences, Toulouse (1999).  
Advisor: HA Jakobsen (Norwegian Institute of Science and Technology, Trondheim)  
BEng, Chemical Engineering, National Institute of Applied Sciences, Toulouse (1999).

### PROFESSIONAL POSITIONS

Assistant Professor, Department of Civil and Environmental Engineering and Princeton Environmental Institute, Princeton University (2015-present).  
Research Scientist (career-track), Earth Sciences Division, Lawrence Berkeley National Laboratory (2009-2014).  
Postdoctoral Scholar, Earth Sciences Division, Lawrence Berkeley National Laboratory (2005-2009). Advisor: G Sposito  
Visiting postdoctoral scholar, Department of Geophysical Sciences, University of Chicago (2008).  
Advisor: FM Richter

### HONORS & AWARDS

NSF CAREER Award, US National Science Foundation (2018).  
Winner, DOE Life at the Frontiers of Energy Research Video Competition (2011).  
Joseph Dias & Eugene Henry Doctoral Fellowships, CEE Department, UC Berkeley (2000, 2002).  
Doctoral Fellowship, French Agency for the Management of Radioactive Waste (1999-2002).  
Leonardo Scholarship, European Union (1999).

### EXTRAMURAL FUNDING (since January 2015)

National Science Foundation, Division of Earth Sciences, Hydrologic Sciences Program, CAREER Award, “Coupled Hydrology and Mechanics of Fine-Grained Soils and Sedimentary Rocks,” 2018-2023; \$400,000 awarded to Bourg (PI).  
Department of Energy, Office of Science, Office of Basic Energy Sciences, Geosciences Program grant, “Nanoscale Basis of the Permeability of Fine-Grained Sedimentary Rocks,” 2018-2021; \$495,054 awarded to Bourg (PI).  
BP International, “A Carbon Mitigation Initiative,” 2016-2020 (Directors: S Pacala, R Socolow); Bourg joined the center as a co-PI in 2016; \$125,000 awarded to Bourg during 2016-2018.  
Department of Energy, Office of Science, Office of Basic Energy Sciences, Energy Frontiers Research Center (EFRC) Program grant, “Center for Nanoscale Controls on Geologic CO<sub>2</sub> (NCGC),” 2014-2018 (Director: DJ DePaolo); \$612,500 awarded to Bourg during 2015-2018.  
Department of Energy, Office of Science, Office of Basic Energy Sciences, Geosciences Program grant, “The Effect of Salinity on Geochemical Processes in Confined Aqueous Fluids,” 2014-2017 (lead PI: B Gilbert; co-PIs: IC Bourg, J Banfield, CI Steefel, KG Knauss, TK Tokunaga); \$369,164 awarded to Bourg during 2015-2017.

### BOOKS

Tournassat C, Steefel CI, Bourg IC, Bergaya F (Eds.) *Natural and Engineered Clay Barriers*, Developments in Clay Science, Vol 6, Elsevier (2015).  
Smit B, Reimer JA, Oldenburg CM, Bourg IC. *Introduction to Carbon Capture and Sequestration*, The Berkeley Lectures on Energy, Vol 1, Imperial College Press (2014).

DePaolo DJ, Cole DR, Navrotsky A, Bourg IC (Eds) *Geochemistry of Geologic CO<sub>2</sub> Sequestration*, Reviews in Mineralogy and Geochemistry, Vol 77, Mineralogical Society of America (2013).

## PEER-REVIEWED PUBLICATIONS

- Collin M, Gin S, Dazas B, Mahadevan T, Du J, Bourg IC. Molecular dynamics simulations of water structure and diffusion in a 1-nm-diameter silica nanopore as a function of surface charge and alkali metal counterion identify. *Journal of Physical Chemistry C* 122, 17764-17776 (2018).
- Okumura M, Kerisit S, Bourg IC, Lammers LN, Ikeda T, Sassi M, Rosso K, Machida M. Radiocesium interaction with clay minerals: Theory and simulation advances post-Fukushima. *Journal of Environmental Radioactivity* 189, 135-145 (2018).
- Gadikota G, Dazas B, Rother G, Cheshire MC, Bourg IC. Hydrophobic solvation of gases (CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>, noble gases) in clay interlayer nanopores. *Journal of Physical Chemistry C* 121, 26539-26550 (2017). [2018 Best Paper Award for Postdoctoral Fellows of the Carbon Mitigation Initiative]
- Bourg IC, Ajo-Franklin JB. Clay, water, and salt: Controls on the permeability of fine-grained sedimentary rocks. *Accounts of Chemical Research* 50, 2067-2074 (2017).
- Bourg IC, Lee SS, Fenter P, Tournassat C. Structure and energetics of the Stern layer at mica-water interfaces. *Journal of Physical Chemistry C* 121, 9402-9412 (2017).
- Lammers LN, Bourg IC, Okumura M, Kolluri K, Sposito G, Machida M. Molecular dynamics simulations of cesium adsorption on illite nanoparticles. *Journal of Colloid and Interface Science* 490, 608-620 (2017).
- Tournassat C, Davis JA, Chiaberge C, Grangeon S, Bourg IC. Modeling the acid-base properties of montmorillonite edge surfaces. *Environmental Science and Technology* 50, 13436-13445 (2016).
- Tournassat C, Bourg IC, Holmboe M, Sposito G, Steefel CI. Molecular dynamics simulations of anion exclusion in clay interlayer nanopores. *Clays and Clay Minerals* 64, 374-388 (2016).
- Bacle P, Dufreche J-F, Rotenberg B, Bourg IC, Marry V. Modeling the transport of water and ionic tracers in a micrometric clay sample. *Applied Clay Science* 123, 18-28 (2016).
- Tinnacher RM, Holmboe M, Tournassat C, Bourg IC, Davis JA. Ion adsorption and diffusion in smectite: Molecular, pore, and continuum scale views. *Geochimica et Cosmochimica Acta* 177, 130-149 (2016).
- Bourg IC. Sealing shales versus brittle shales: A sharp threshold in the material properties and energy technology uses of fine-grained sedimentary rocks. *Environmental Science and Technology Letters* 2, 255-259 (2015).
- Bourg IC, Beckingham L, DePaolo DJ. The nanoscale basis of CO<sub>2</sub> trapping for geologic storage. *Environmental Science and Technology* 49, 10265-10284 (2015).
- Bourg IC, Tournassat C. Self-diffusion of water and ions in clay barriers. In: *Natural and Engineered Clay Barriers* (C Tournassat, CI Steefel, IC Bourg, F Bergaya, eds.), Developments in Clay Science, Vol. 6, Elsevier, Chapter 6 (2015).
- Tournassat C, Bourg IC, Steefel CI, Bergaya F. General surface properties of clay minerals. In: *Natural and Engineered Clay Barriers* (C Tournassat, CI Steefel, IC Bourg, F Bergaya, eds.), Developments in Clay Science, Vol. 6, Elsevier, Chapter 1 (2015).
- Chagneau A, Tournassat C, Steefel CI, Bourg IC, Gaboreau S, Esteve I, Kupick T, Claret F, Schafer T. Complete restriction of <sup>36</sup>Cl<sup>-</sup> diffusion by celestite precipitation in densely compacted illite. *Environmental Science and Technology Letters* 2, 139-143 (2015).
- Holmboe M, Bourg IC. Molecular dynamics simulations of water and sodium diffusion in smectite interlayer nanopores as a function of pore size and temperature. *Journal of Physical Chemistry C* 118, 1001-1013 (2014).

- Eiler JM, Bergquist B, Bourg IC, Cartigny P, Farquhar J, Gagnon AC, Guo W, Halevy I, Hofmann AE, Levin N, Schauble EA, Stolper D. Frontiers of stable isotope geoscience. *Chemical Geology* 372, 119-143 (2014).
- Hamm LM, Bourg IC, Wallace AF, Rotenberg B. Molecular simulation of CO<sub>2</sub>- and CO<sub>3</sub>-brine-mineral systems. In: *Geochemistry of Geologic CO<sub>2</sub> Sequestration* (DJ DePaolo, DR Cole, A Navrotsky, IC Bourg, eds.), Reviews in Mineralogy and Geochemistry, Vol. 77, Mineralogical Society of America, pp. 189-228 (2013).
- Hofmann AE, Bourg IC, DePaolo DJ. Ion desolvation as a mechanism for kinetic isotope fractionation in aqueous systems. *Proceedings of the National Academy of Sciences of the U.S.A.* 198, 18689-18694 (2012).
- Bourg IC, Steefel CI. Molecular dynamics simulations of water structure and diffusion in silica nanopores. *Journal of Physical Chemistry C* 116, 11556-11564 (2012).
- Nielsen LC, Bourg IC, Sposito G. Predicting CO<sub>2</sub>-water interfacial tension under pressure and temperature conditions of geologic CO<sub>2</sub> storage. *Geochimica et Cosmochimica Acta* 81, 28-38 (2012).
- Bourg IC, Sposito G. Molecular dynamics simulations of the electrical double layer on smectite surfaces contacting concentrated mixed electrolyte (NaCl-CaCl<sub>2</sub>) solutions. *Journal of Colloid and Interface Science* 360, 701-715 (2011).
- Bourg IC, Sposito G. Ion exchange phenomena. In: *Handbook of Soil Sciences, Properties and Processes*, 2<sup>nd</sup> ed. (PM Huang, Y Li, ME Sumner, eds.), CRC Press, Boca Raton, Chapter 16 (2011).
- Bourg IC, Sposito G. Connecting the molecular scale to the continuum scale for diffusion processes in smectite-rich porous media. *Environmental Science and Technology* 44, 2085-2091 (2010).
- Bourg IC, Richter FM, Christensen JN, Sposito G. Isotopic mass-dependence of alkali metal cation diffusion coefficients in water. *Geochimica et Cosmochimica Acta* 74, 2249-2256 (2010).
- Bourg IC, Sposito G. Isotopic fractionation of noble gases by diffusion in liquid water: Molecular dynamics simulations and hydrologic applications. *Geochimica et Cosmochimica Acta* 72, 2237-2247 (2008).
- Bourg IC, Sposito G, Bourg ACM. Modeling the diffusion of Na<sup>+</sup> in compacted water-saturated Na-bentonite as a function of pore water ionic strength. *Applied Geochemistry* 23, 3635-3641 (2008).
- Bourg IC. Comment on "Modeling sulfur isotope fractionation and differential diffusion during sulfate reduction in sediments of the Cariaco Basin" by MA Donahue, JP Werne, C Meile and TW Lyons. *Geochimica et Cosmochimica Acta* 72, 5852-5854 (2008).
- Bourg IC, Sposito G. Molecular dynamics simulation of kinetic isotope fractionation during the diffusion of ionic species in liquid water. *Geochimica et Cosmochimica Acta* 71, 5583-5589 (2007).
- Bourg IC, Sposito G, Bourg ACM. Modeling the acid-base surface chemistry of montmorillonite. *Journal of Colloid and Interface Science* 312, 297-310 (2007).
- Bourg IC, Sposito G, Bourg ACM. Modeling cation diffusion in compacted water-saturated Na-bentonite at low ionic strength. *Environmental Science and Technology* 41, 8118-8122 (2007).
- Bourg IC, Sposito G, Bourg ACM. Tracer diffusion in compacted water-saturated bentonite. *Clays and Clay Minerals* 54, 363-374 (2006).
- Bourg IC, Bourg ACM, Sposito G. Modeling diffusion and adsorption in compacted bentonite: a critical review. *Journal of Contaminant Hydrology* 61, 293-302 (2003).

**INVITED LECTURES** (presenting author in bold)

Dr Bourg has given 58 invited lectures. His collaborators have given 6 invited lectures on which he was listed as a co-author, to the best of his knowledge.

**Bourg IC.** Molecular basis of soil carbon protection by mineral surfaces. Goldschmidt conference, Boston, August 2018. (ICB invited by K Rosso, Pacific Northwest National Lab)

Dazas B, **Gilbert B**, Zarzycki P, Bourg IC. Dielectric relaxation and static dielectric constant of confined aqueous solutions. Goldschmidt conference, Boston, August 2018.

**Lee SS**, Koishi A, Bourg IC, Fenter P. Intrinsic complexity of ion adsorption structures at the muscovite (001)-brine interface. Goldschmidt conference, Boston, August 2018.

**Bourg IC.** Impact of clay swelling on fluid flow in soils and sedimentary rocks. Soft Materials Coffee Hour, Department of Chemical and Biological Engineering, Princeton University, June 2018. (host: S Datta)

**Bourg IC.** Fundamental controls on soil carbon storage. Clay Minerals Society (CMS) annual meeting, Urbana-Champaign, June 2018. (ICB invited by D Cole, Ohio State U)

**Bourg IC.** Clay, water, and salt: Controls on the hydrology and mechanics of fine-grained soils and sedimentary rocks. Geodynamics seminar series, Lamont-Doherty Earth Observatory, May 2018. (hosts: C McCarthy and P Kelemen)

Gadikota G, Dazas B, Rother G, Cheshire M, **Bourg IC.** Solubility of gases (CO<sub>2</sub>, CH<sub>4</sub>, noble gases) in nanoconfined water. American Chemical Society Spring meeting, New Orleans, March 2018. (ICB invited by J Kirkpatrick, Michigan State U)

**Bourg IC.** Clay, water, and salt: Controls on the hydrology and mechanics of fine-grained soils and sedimentary rocks. Environmental Geology and Geochemistry seminar, Department of Geosciences, Princeton University, February 2018. (host: S Myneni)

**Lee SS**, Bracco JN, Bourg IC, Stack AG, Fenter P. Hydration structure of solid-water interfaces. Telluride workshop on Clathrate Hydrates Fundamentals, Telluride, June 2017.

**Bourg IC**, Lee SS, Fenter P, Tournassat C. Structure and energetics of the Stern layer at mica-water interfaces. Mid-Atlantic Regional Meeting, American Chemical Society, Hershey, June 2017. (ICB invited by R Hinrichs, Drew U)

**Gilbert B**, Pradeep P, Schuck JP, Sokaras D, Bourg IC, Tokunaga TK. Van der Waals wetting forces relevant to geologic carbon sequestration from inelastic X-ray scattering. American Chemical Society Spring meeting, San Francisco, April 2017.

**Bourg IC.** How clay minerals control fluid flow in the subsurface. Pierce seminar series, Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, December 2016. (host: R Juanes)

**Bourg IC**, Tournassat C. Acid-base reactivity of smectite edge surfaces. American Chemical Society Fall meeting, Philadelphia, August 2016. (ICB invited by N Birkner, UC Merced)

**Bourg IC**, Tinnacher RM, Holmboe M, Tournassat C. Water and ion diffusion in Na-smectite clay barriers. American Chemical Society Fall meeting, Philadelphia, August 2016. (ICB invited by E Elzinga, Rutgers U)

**Bourg IC.** Water, ions, and clay: a molecular-scale view. Division of Energy and Environmental Systems, Hokkaido University, July 2016. (host: N Watanabe, Hokkaido U)

Lammers LN, **Bourg IC**, Okumura M, Kolluri K, Sposito G, Machida M. MD simulations of Cs<sup>+</sup> adsorption on illite nanoparticles. Goldschmidt conference, Yokohama, June 2016. (ICB invited by SS Lee, Argonne National Lab)

Lammers LN, **Bourg IC**, Okumura M, Kolluri K, Sposito G, Machida M. MD simulations of Cs<sup>+</sup> adsorption on illite nanoparticles. Clay Minerals Society annual meeting, Atlanta, June 2016. (ICB invited by J Greathouse, Sandia National Labs)

**Bourg IC.** Mineralogical controls on shale properties and low-carbon energy uses. Department of Energy, Environmental, and Chemical Engineering, Washington University in St. Louis, March 2016. (host: D Giammar)

- Bourg IC.** MD simulations of Cs<sup>+</sup> adsorption on illite and mica. Department of Earth and Planetary Sciences, Washington University in St. Louis, March 2016. (host: J Catalano)
- Bourg IC,** Lammers LN, Kolluri K, Okumura M, Sposito G, Machida M. Molecular dynamics simulations of cesium adsorption on illite. American Chemical Society Spring meeting, San Diego, March 2016. (ICB invited by Y Yang, U Nevada-Reno, and J Fein, U of Notre Dame)
- DePaolo DJ,** Lammers LN, Watkins J, De Yoreo J, Bourg IC, Ryerson R, Hofmann AE. Isotopes and impurities as microprobes of the mineral surface dynamics of calcite growth. American Chemical Society Spring meeting, San Diego, March 2016.
- Bourg IC.** Mineralogical controls on shale properties and low-carbon energy uses. Department of Geosciences, University of Delaware, February 2016. (host: N Sturchio)
- Bourg IC.** Mineralogical controls on shale properties and low-carbon energy uses. Geodynamics seminar series, Lamont-Doherty Earth Observatory, February 2016. (host: N Zakharova)
- Bourg IC,** Beckingham LE, DePaolo DJ. Sealing shales vs. brittle shales: A threshold in the properties and uses of fine-grained sedimentary rocks. American Geophysical Union Fall meeting, San Francisco, December 2015. (ICB invited by J Heath, Sandia National Labs)
- Bourg IC.** Molecular basis of kinetic isotope effects. Goldschmidt conference, Prague, August 2015. (ICB invited by J Druhan, UIUC, and K Maher, Stanford U) **[Keynote presentation]**
- Bourg IC,** Lee SS, Fenter P. Metal and water adsorption at mica-water interfaces. Goldschmidt conference, Prague, August 2015. (ICB invited by J Catalano, Washington U, A Stack, Oak Ridge National Lab, and JF Boily, Umeå U)
- Bourg IC.** Adsorption and diffusion in silica nanopores. American Chemical Society Spring meeting, Denver, March 2015. (ICB invited by A Fernandez-Martinez, U of Grenoble, and A Stack, Oak Ridge National Lab)
- Bourg IC,** Lee SS, Fenter P. Alkali metal adsorption at mica-water interfaces. American Chemical Society Spring meeting, Denver, March 2015. (ICB invited by SS Lee, Argonne National Lab, A Ilgen, Sandia National Labs, and S Mason, U Iowa)
- Bourg IC.** Advection and diffusion in clayey media. Swedish Radioactive Waste Management agency (SKB), 32<sup>nd</sup> International Task Force GWFTS (modeling of GroundWater Flow and Transport of Solutes) meeting, Berkeley, December 2014. (ICB invited by U Mäder, U of Bern)
- Bourg IC,** Holmboe M. Atomistic-level views of clay-water interfaces. Swedish Radioactive Waste Management agency (SKB), 32<sup>nd</sup> International Task Force GWFTS (modeling of GroundWater Flow and Transport of Solutes) meeting, Berkeley, December 2014. (ICB invited by S Finsterle, Lawrence Berkeley National Lab)
- Bourg IC,** Tournassat C. MD simulations of cation adsorption at mica-water interfaces. Molecular Foundry users' meeting, Lawrence Berkeley National Laboratory, August 2014. (ICB invited by S Harris, Lawrence Berkeley National Lab)
- Bourg IC, **Sposito G.** Molecular simulations of water in clay mineral nanopores. American Chemical Society Fall meeting, San Francisco, August 2014.
- Bourg IC.** The nanoscale basis of geologic carbon sequestration. Workshop on Characterization of Nanoporous Materials, Stanford University, August 2014. (ICB invited by J Wilcox, Stanford U)
- Bourg IC,** Tournassat C. MD simulations of cation adsorption at mica-water interfaces. Clay Minerals Society annual meeting, College Station, May 2014. (ICB invited by X Liu, U of Cambridge, and A Kalinichev, Nantes School of Mines)
- Bourg IC,** Tinnacher R, Davis JA, Holmboe M, Tournassat C. Water and ion diffusion in water-saturated Na-smectite at  $\rho_b = 0.75 \text{ kg dm}^{-3}$ . Clay Minerals Society annual meeting, College Station, May 2014. (ICB invited by N Qafoku and J Neeway, Pacific Northwest National Lab)
- Bourg IC.** Liquid water at interfaces: new insights from molecular scale studies. Department of Civil and Environmental Engineering, Princeton University, April 2014. (host: J Smith)

- Bourg IC.** Liquid water at interfaces: new insights from molecular scale studies. Department of Earth and Environmental Sciences, Rensselaer Polytechnic Institute, March 2014. (host: F Spear)
- Bourg IC.** Liquid water at interfaces: new insights from molecular scale studies. Center for Isotope Geochemistry seminar series, Department of Earth and Planetary Sciences, UC Berkeley, February 2014. (host: A Basu)
- Bourg IC, Hofmann AE, Sposito G, DePaolo DJ.** Molecular-scale basis of kinetic isotope effects associated with diffusion and ligand exchange in liquid water. American Chemical Society Spring meeting, New Orleans, April 2013. (ICB invited by A Hofmann, Lawrence Berkeley National Lab, A Stack, Oak Ridge National Lab, L Criscenti, Sandia National Lab, and S Kerisit, Pacific Northwest National Lab)
- Bourg IC.** The nanoscience of geologic CO<sub>2</sub> sequestration. Department of Geology, University of Illinois at Urbana-Champaign, November 2012. (host: T Johnson)
- Bourg IC.** Water in the nanopores of clays, cement, and silica gels. International Seminar Series on Environmental Radioactivity, Division of Energy and Environmental Systems, Hokkaido University, November 2012. (host: T Kozaki)
- Bourg IC.** Water and clay: MD simulations and their relevance to solute migration in argillaceous media. 5<sup>th</sup> International Meeting on Clays in Natural and Engineered Barriers for Radioactive Waste Confinement, Montpellier, October 2012. (ICB invited by B Rotenberg, U of Paris, and A Kalinichev, Nantes School of Mines) **[Plenary keynote presentation]**
- Bourg IC.** The nanoscience of geologic CO<sub>2</sub> sequestration. Department of Civil and Environmental Engineering, University of Connecticut, September 2012. (host: A MacKay)
- Bourg IC.** Nanoscale basis of CO<sub>2</sub>-brine multiphase flow and geochemistry in CO<sub>2</sub> storage repositories. Center for Frontiers of Subsurface Energy Security (CFSES), Sandia National Laboratories, June 2012. (host: R Cygan)
- Bourg IC.** Nanoscale basis of CO<sub>2</sub>-brine multiphase flow and geochemistry in CO<sub>2</sub> storage repositories. Geophysical Laboratory, Carnegie Institute in Washington, DC, June 2012. (host: T Strobel)
- Bourg IC, Sposito G.** MD simulations of the electrical double layer on smectite clay surfaces. APS workshop on Metal Ion Adsorption at Interfaces, APS/CNM/EMC users' meeting, Argonne National Laboratory, May 2012. (ICB invited by P Fenter, Argonne National Lab)
- Bourg IC.** Nanoscale CO<sub>2</sub>-brine-mineral interactions in carbon dioxide storage repositories. Young Engineers + Scientists Symposium, Berkeley, March 2012. (ICB invited by T Deschamps, French Consulate in San Francisco)
- Bourg IC.** Nanopore processes in sealing caprocks of carbon dioxide storage repositories. Symposium on Application of Nano-geosciences in Petroleum Engineering, Kyoto University, December 2011. (hosts: Y Liang and T Matsuoka)
- Bourg IC.** Water, ions and clay minerals. Energy and Environmental Systems seminar series, Hokkaido University, December 2011. (host: T Kozaki)
- Bourg IC.** Molecular dynamics simulations of the electrical double layer on smectite clay surfaces. Goldschmidt conference, Prague, August 2011. (ICB invited by C Steefel, Lawrence Berkeley National Lab)
- Bourg IC.** Nanoscale views of water and solutes in low-permeability porous media. Department of Civil and Environmental Engineering, Pennsylvania State University, February 2011. (host: W Burgos)
- Bourg IC.** Kinetic isotope fractionation during diffusion in water. US DOE workshop on the Chemistry of Novel Isotope Effects in the Geosciences, San Francisco, December 2010. (ICB invited by J Eiler, CalTech)

- Bourg IC.** Minerals, brines, and CO<sub>2</sub>: molecular modeling and carbon storage. Berkeley Seismology Lab seminar series, Department of Earth and Planetary Sciences, UC Berkeley, October 2010. (host: B Romanowicz)
- Bourg IC.** Molecular dynamics modeling in isotope geochemistry. Center for Isotope Geochemistry seminar series, Department of Earth and Planetary Sciences, UC Berkeley, April 2010. (host: B Peterson)
- Bourg IC.** Molecular modeling: applications to geochemistry and hydrology. Ecosystem Sciences seminar series, Department of Environmental Sciences, Policy, and Management, UC Berkeley, March 2010. (host: M Kelly)
- Bourg IC.** Molecular modeling: applications to geochemistry and hydrology. Geochemistry Department, Lawrence Berkeley National Laboratory, August 2009. (host: C Steefel)
- Bourg IC,** Sposito G., Refson K, Richter F. Diffusion near clay surfaces: Bridging the nanopore and continuum scales. American Chemical Society Spring meeting, Salt Lake City, March 2009. (ICB invited by B Bickmore, Brigham Young U)
- Bourg IC.** Cations and clay minerals: New insights from molecular- and pore-scale studies. Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, March 2008. (host: R Juanes)
- Bourg IC.** Cations and clay minerals: New insights from molecular- and pore-scale studies. Department of Geology, Federal Polytechnic Institute of Zurich (ETHZ), January 2008. (host: S Löw)
- Bourg IC,** Sposito G. Kinetic isotope fractionation during the diffusion of solutes in liquid water. DOE Workshop on Molecular Dynamics and Structure of Geofluids, Berkeley, December 2007. (ICB invited by L Stixrude, U Michigan)
- Bourg IC.** Modeling montmorillonite acid-base titration. European Union workshop on Surface Reactions & Electrical Interfacial Layer, Opatija, October 2007. (ICB invited by J Lützenkirchen, Karlsruhe Inst Technol)
- Bourg IC,** Sposito G. Molecular diffusion in water and smectite nanopores. LGIT-ILL workshop on Neutron Scattering and Molecular Dynamics in Environmental Sciences, University of Grenoble, January 2007. (ICB invited by L Charlet, U Grenoble)
- Bourg IC,** Sposito G, Bourg ACM. Diffusion of water and sodium in water-saturated Na-bentonite. International Workshop on Waste Management, Hokkaido University, August 2005. (host: T Kozaki)
- Bourg IC,** Sposito G, Bourg ACM. Diffusion of water and sodium in water-saturated Na-bentonite. International Clay Conference, Tokyo, August 2005. (ICB invited by T Kozaki, Hokkaido U)

**CONTRIBUTED PAPERS AT SCIENTIFIC MEETINGS** (presenting author in bold)

- Carrillo FJ,** Bourg IC. Hydro-chemo-mechanically coupled computational fluid and solid dynamics in deformable porous media. Goldschmidt conference, Boston, August 2018.
- Koishi A,** Lee SS, Fenter P, Fernandez-Martinez A, Michot L, Bourg IC. Surface hydrophobicity and properties of interfacial water. Goldschmidt conference, Boston, August 2018.
- Shen X,** Bourg IC. Free energy of interaction of two smectite clay nanoparticles in liquid water. Goldschmidt conference, Boston, August 2018.
- Sun EWH,** Bourg IC. Molecular dynamics simulation prediction of quartz wetting by water and supercritical CO<sub>2</sub>. Goldschmidt conference, Boston, August 2018.
- Underwood TR,** Bourg IC. Emergent properties of clay: Molecular dynamics simulations of nanoconfined water in the clay matrix. Goldschmidt conference, Boston, August 2018.
- Willemsen J,** Myneni S, Bourg IC. Metadynamics based molecular dynamics simulation and experimental study of the adsorption of phthalate esters on smectite clay surfaces. Goldschmidt conference, Boston, August 2018.

- Underwood T, **Bourg IC**. Molecular dynamics simulations of water-saturated Na-smectite clay during one-dimensional consolidation. US DOE, Office of Basic Energy Sciences, Geosciences Program PI meeting, Washington DC, August 2018.
- Dzas B, Colla C, Prus M, Kedra-Krolik K, Zarzycki P, Li A, Castro RHR, Bourg IC, **Gilbert B**. The dynamics of confined aqueous solutions. US DOE, Office of Basic Energy Sciences, Geosciences Program PI meeting, Washington DC, August 2018.
- Bourg IC**, Lee SS, Fenter P. The Stern layer at mica-water interfaces. Gordon Research Conference on Water and Aqueous Solutions, Holderness, July 2018.
- Underwood TR**, Bourg IC. Interfacial water in the clay matrix – A molecular dynamics study. Gordon Research Conference on Water and Aqueous Solutions, Holderness, July 2018.
- Koishi A**, Lee SS, Fenter P, Fernandez-Martinez A, Michot L, Bourg IC. Effect of fluorine substitution in phlogopite mica on surface hydrophobicity and properties of interfacial water. Gordon Research Conference on Water and Aqueous Solutions, Holderness, July 2018.
- Carrillo FJ**, Bourg IC. A framework toward modeling hydro-chemo-mechanical couplings in deformable porous media. Gordon Research Conference on Flow and Transport in Permeable Media, Newry, July 2018.
- Underwood TR**, Bourg IC. Properties of fine-grained clay-rich sedimentary rocks. Gordon Research Conference on Flow and Transport in Permeable Media, Newry, July 2018.
- Bourg IC**. Clay, water, and salt: Controls on water flow in fine-grained sedimentary rocks. Computational Methods in Water Resources (CMWR) conference, Saint-Malo, June 2018.
- Carrillo FJ**, Bourg IC. Coupled solid-fluid dynamics in heterogeneous porous media. Computational Methods in Water Resources (CMWR) conference, Saint-Malo, June 2018.
- Underwood TR**, Bourg IC. Properties of fine-grained clay-rich sedimentary rocks from large scale molecular dynamics simulations. Computational Methods in Water Resources (CMWR) conference, Saint-Malo, June 2018.
- Bourg IC**. Fundamental controls on soil carbon storage. Carbon Mitigation Initiative (CMI) annual meeting, London, April 2018.
- Lee SS**, Bracco JN, Bourg IC, Stack AG, Fenter P. Hydration structure of mineral-water interfaces. American Chemical Society Spring meeting, New Orleans, March 2018.
- Rother G**, Cole D, Bourg IC, Cheshire M, Vlcek L. Gas and supercritical fluid adsorption at mineral surfaces, in narrow pores, and to swelling clays: Impacts of hydration and fluid identity. American Chemical Society Spring meeting, New Orleans, March 2018.
- Shen X**, Bourg IC. Free energy of interaction of two smectite clay nanoparticles in liquid water. American Chemical Society Spring meeting, New Orleans, March 2018.
- Sun EWH**, Bourg IC. Impact of small organic molecules on the wettability of quartz by brine versus CO<sub>2</sub>. American Chemical Society Spring meeting, New Orleans, March 2018.
- Underwood TR**, Bourg IC. Properties of clay-rich fine-grained sedimentary rocks from large-scale molecular dynamics simulations. American Chemical Society Spring meeting, New Orleans, March 2018.
- Willemsen J**, Myneni S, Bourg IC. Metadynamics based molecular dynamics simulation and experimental study of the adsorption of phthalate esters on smectite clay surfaces. American Chemical Society Spring meeting, New Orleans, March 2018.
- Bourg IC**. Nanoscale controls on soil carbon storage. Carbon Mitigation Initiative seminar series, Princeton Environmental Institute, Princeton University, November 2017.
- Bourg IC**. Clay, water, and salt: Controls on the permeability of fine-grained sedimentary rocks. 7<sup>th</sup> International Meeting on Clays in Natural and Engineered Barriers for Radioactive Waste Confinement, Davos, September 2017. [**Abstract graphic on the cover page of the conference booklet**]
- Bourg IC**. Clay, water, and salt: Controls on the permeability of fine-grained sedimentary rocks. Goldschmidt conference, Paris, August 2017.



- Willemssen J**, Bourg IC. Molecular dynamics simulation and experimental study of the adsorption of phthalate esters on clay surfaces. Goldschmidt conference, Paris, August 2017.
- Bourg IC**, Lee SS, Fenter P, Tournassat C. Stern layer structure and energetics at mica-water interfaces. US DOE, Office of Basic Energy Sciences, Geosciences Program PI meeting, Washington DC, August 2017.
- Gadikota G, Dazas B, Rother G, Cheshire M, **Bourg IC**. Solubility of gases in clay interlayer nanopore water. EFRC PI meeting, US Department of Energy, Washington DC, July 2017.
- Amaral V**, Dazas B, Bourg IC. Cesium adsorption on illite: Characterizing the slow adsorption sites. American Chemical Society Spring meeting, San Francisco, April 2017. **[Talk given by a senior thesis student]**
- Gadikota G**, Dazas B, Bourg IC. Molecular dynamics simulation prediction of the solubility of gases (CO<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>, noble gases) in nano-confined water. American Chemical Society Spring meeting, San Francisco, April 2017.
- Willemssen J**, Myneni S, Bourg IC. Molecular dynamics simulation and experimental study of the adsorption of phthalate esters on clay surfaces. American Chemical Society Spring meeting, San Francisco, April 2017.
- Gadikota G, Dazas B, **Bourg IC**. Adsorption of dissolved gases (CH<sub>4</sub>, CO<sub>2</sub>, H<sub>2</sub>, noble gases) by water-saturated smectite clay minerals. American Geophysical Union Fall meeting, San Francisco, December 2016.
- Kulasinski K**, Bourg IC, Lammers LN. Investigation of frayed edge site formation in high structural charge clay minerals by molecular dynamics simulation. American Geophysical Union Fall meeting, San Francisco, December 2016.
- Bourg IC**. Sealing shales vs. brittle shales: A threshold in the properties and uses of fine-grained sedimentary rocks. Materials Research Society annual meeting, Boston, November 2016.
- Lammers LN, **Bourg IC**, Okumura M, Kolluri K, Sposito G, Machida M. MD simulations of Cs<sup>+</sup> adsorption on illite nanoparticles. Materials Research Society annual meeting, Boston, November 2016.
- Gadikota G**, Dazas B, Bourg IC. Molecular dynamics simulations of clay-water-gas interactions for sustainable energy and environment. American Chemical Society Fall meeting, Philadelphia, August 2016.
- Bourg IC**. Permeability and mechanics of shale and mudstone. Gordon Research Conference on Flow and Transport in Permeable Media, Barcelona, August 2016.
- Gilbert B**, Tester C, Comolli L, Dazas B, Chagneau A, Zarzycki P, Tournassat C, Bourg IC, Steefel C, Banfield J. Confined water in smectite. US DOE, Office of Basic Energy Sciences, Geosciences Program PI meeting, Washington DC, August 2016.
- Holmboe M**, Bourg IC, Tournassat C. Anion exclusion in hydrated clay nanopores studied by molecular dynamics simulation. American Chemical Society Fall meeting, Philadelphia, August 2016.
- Lee SS**, Bourg IC, Fenter P. Distribution of monovalent cations adsorbed at the muscovite (001) – water interface: Comparison between X-ray reflectivity and molecular dynamics simulations. American Chemical Society Fall meeting, Philadelphia, August 2016.
- Lee SS**, Bourg IC, Fenter P. Understanding cation adsorption on mica using X-ray reflectivity and molecular dynamics simulations. Goldschmidt conference, Yokohama, June 2016.
- Dazas B**, Gilbert B, Bourg IC. Broadband dielectric spectroscopy study of smectites, collation of simulations and experiments. Goldschmidt conference, Yokohama, June 2016.
- Bourg IC**. The permeability of fine-grained sedimentary rocks. Clay Minerals Society annual meeting, Atlanta, June 2016.
- Bourg IC**. Mineralogical controls on shale permeability. Carbon Mitigation Initiative (CMI) annual meeting, London, April 2016.

- Bourg IC**, Beckingham LE, DePaolo DJ, Swift AM, Cole DR. From fine-grained rocks to low-carbon energy. EFRC PI meeting, US Department of Energy, Washington DC, October 2015.
- Tournassat C**, Bourg IC, Steefel CI. Breakdown of the modified Gouy-Chapman model for clay surfaces in equilibrium with a  $\text{CaCl}_2$  electrolyte: a molecular dynamics study. 6<sup>th</sup> International Meeting on Clays in Natural and Engineered Barriers for Radioactive Waste Confinement, Brussels, March 2015.
- Tinnacher R, Holmboe M, Tournassat C, **Bourg IC**, Davis JA. Diffusion of water and ions in water-saturated Na-montmorillonite. Réunion des Sciences de la Terre, Pau, October 2014.
- Bourg IC**, Tournassat C. MD simulations of cation adsorption at mica-water interfaces. American Chemical Society Fall meeting, San Francisco, August 2014.
- Tournassat C**, Bourg IC, Steefel CI. Quantification of the breakdown of modified Gouy-Chapman model for 2:1 salt background electrolyte: a molecular dynamic study. American Chemical Society Fall meeting, San Francisco, August 2014.
- Tinnacher R**, Holmboe M, Davis JA, Tournassat C, Bourg IC. Impacts of pore structure and diffusion-accessible porosity for calcium-bromide diffusion in sodium-montmorillonite. American Chemical Society Fall meeting, San Francisco, August 2014.
- Bourg IC**. Molecular dynamics simulations of ion adsorption at mica-water interfaces. Goldschmidt conference, Sacramento, June 2014.
- Holmboe M**, Bourg IC. Clay mineral hydration studied with *in silico* techniques. Goldschmidt conference, Sacramento, June 2014.
- DePaolo DJ**, Christensen JN, Kennedy BM, Conrad ME, Bourg IC. Kinetic isotope fractionation during mineral growth and fluid phase transport. US DOE, Office of Basic Energy Sciences, Geosciences Program PI meeting, Washington DC, May 2014.
- Bourg IC**, Sposito G. Clay minerals and cesium: Proposed MD simulation research. Japan Atomic Energy Agency, Tokyo, March 2014.
- Hamm LM, **Bourg IC**, Wallace AF, Rotenberg B. Molecular simulation of  $\text{CO}_2$ - and  $\text{CO}_3$ -brine-mineral systems. Mineralogical Society of American short course on the Geochemistry of Geologic  $\text{CO}_2$  Sequestration, Berkeley, December 2013.
- Liu Y, **Bourg IC**. Wettability of silica by brine vs.  $\text{CO}_2$ : The nanoscale view. American Geophysical Union Fall meeting, San Francisco, December 2013.
- Bourg IC**, Holmboe M, Steefel CI, Sposito G. Pore-scale view of engineered clay barriers for HLRW storage. Clay Minerals Society annual meeting, Urbana-Champaign, October 2013.
- Bourg IC**, Holmboe M, Christensen JN, Sposito G. Isotopic fractionation by diffusion in clay barriers. Clay Minerals Society annual meeting, Urbana-Champaign, October 2013.
- Lee SS**, Fenter P, Nagy KL, Sturchio NC, Hamm LM, Bourg IC. In-situ measurements of cation adsorption and desorption kinetics at the muscovite (001)-water interface. American Chemical Society Fall meeting, Indianapolis, September 2013.
- Liu Y, **Bourg IC**. Wettability of silica by brine vs.  $\text{CO}_2$ : The nanoscale view. EFRC PI meeting, US Department of Energy, Washington DC, July 2013.
- Bourg IC**. Geochemistry and seal integrity in GCS. 12<sup>th</sup> annual Carbon Capture, Utilization & Sequestration conference, Pittsburgh, May 2013.
- Holmboe M**, Bourg IC. Interlayer diffusion in hydrated smectites – a molecular dynamics study. American Chemical Society Spring meeting, New Orleans, April 2013.
- Hoffmann AE**, Bourg IC, Christensen JC, DePaolo DJ. Diffusion-driven isotopic fractionation of ionic species in  $\text{D}_2\text{O}$  and methanol. American Chemical Society Spring meeting, New Orleans, April 2013.
- Hoffmann AE**, Bourg IC, DePaolo DJ. Isotopic mass dependence of cation desolvation rates in aqueous solution. American Chemical Society Fall meeting, Philadelphia, August 2012.
- Bourg IC**. Molecular-scale basis of the ion exchange selectivity of clay minerals. Goldschmidt conference, Montreal, June 2012.

- Holmboe M**, Bourg IC. Molecular dynamics simulations of two- and three-layer hydrates in smectites. Goldschmidt conference, Montreal, June 2012.
- Sposito G**, Kwon KD, Bourg IC, Refson K. Molecular simulations of geochemical interfaces. American Chemical Society Spring meeting, San Diego, March 2012.
- Bourg IC**, Steefel CI. Molecular dynamics simulations of water confined in silica nanopores. American Geophysical Union Fall meeting, San Francisco, December 2011.
- Fernandez-Martinez A**, Cuello GJ, Bourg IC, Johnson MR, Waychunas GA, Sposito G, Charlet L. Water structure and hydration properties of imogolite nanotubes. Goldschmidt conference, Prague, August 2011.
- Bourg IC**. Nanopore processes in sealing caprocks of carbon dioxide storage repositories. EFR Summit and Forum, US Department of Energy, Washington DC, May 2011.
- Bourg IC**, Sposito G. Adsorption in the electrical double layer at clay-water interfaces. American Geophysical Union Fall meeting, San Francisco, December 2010.
- Nielsen LC**, Bourg IC, Sposito G. Molecular modeling of carbon dioxide-water mixtures under geologic sequestration conditions. Geological Society of America annual meeting, Denver, November 2010.
- Bourg IC**, Sposito G. Electric double layers in saline aquifers: MD simulations of brine-clay interfaces. Goldschmidt conference, Knoxville, June 2010.
- Nielsen LC**, Bourg IC, Sposito G. Molecular dynamics simulations of the supercritical CO<sub>2</sub>-brine interface: predicting geologic CO<sub>2</sub> storage capacities and characteristics. Goldschmidt conference, Knoxville, June 2010.
- Bourg IC**, Sposito G. Ion exchange selectivity of smectites in the ternary system Na<sup>+</sup>-Ca<sup>2+</sup>-CaCl<sup>+</sup>. American Chemical Society Spring meeting, San Francisco, March 2010.
- Bourg IC**, Sposito G. Solute isotope fractionation by diffusion in liquid water. American Geophysical Union Fall meeting, San Francisco, December 2009.
- Bourg IC**, Sposito G. Diffusion of water and solutes near clay surfaces. 12<sup>th</sup> International Conference on the Chemistry and Migration Behavior of Actinides and Fission Products in the Geosphere, Kennewick, September 2009.
- Bourg IC**, Sposito G. Isotopic fractionation by diffusion in liquid water and clay nanopores. Goldschmidt conference, Davos, June 2009.
- Bourg IC**, Kwon KD, Sposito G., Refson K, Richter F. Computational geochemistry: Applications to mineralogy, geochemistry, and hydrology. US DOE, Office of Basic Energy Sciences, Geosciences Program PI meeting, Washington DC, March 2009.
- Bourg IC**, Sposito G. Diffusion in argillaceous media: Bridging the molecular and laboratory scales. American Geophysical Union Fall meeting, San Francisco, December 2008.
- Bourg IC**, Sposito G. Molecular dynamics simulations of kinetic isotope fractionation during the diffusion of solutes in liquid water. American Geophysical Union Fall meeting, San Francisco, December 2007.
- Bourg IC**, Sposito G, Bourg ACM. Modeling the acid-base surface chemistry of montmorillonite. Clay Minerals Society annual meeting, Santa Fe, June 2007.
- Bourg IC**, Sposito G, Bourg ACM. Acid-base titration of montmorillonite. American Chemical Society Fall meeting, San Francisco, September 2006.
- Bourg IC**, Sposito G, Bourg ACM. Diffusion of water and ions in water-saturated bentonite. American Geophysical Union Fall meeting, San Francisco, December 2005.
- Bourg IC**, Sposito G, Bourg ACM. Diffusion of Na<sup>+</sup> and Sr<sup>2+</sup> tracers in compacted, saturated Na-bentonite. 10<sup>th</sup> International Conference on the Chemistry and Migration Behavior of Actinides and Fission Products in the Geosphere, Avignon, September 2005.
- Bourg IC**, Sposito G, Bourg ACM. Diffusion of water tracers in compacted, saturated Na-bentonite. 2<sup>nd</sup> International Meeting on Clays in Natural and Engineered Barriers for Radioactive Waste Confinement, Tours, March 2005.

**Bourg IC**, Bourg ACM, Sposito G. The acid-base titration of montmorillonite. American Geophysical Union Fall meeting, San Francisco, December 2003.

**Bourg IC**, Bourg ACM, Sposito G. Diffusion of water through compacted bentonite clay: a dual porosity approach. American Geophysical Union Fall meeting, San Francisco, December 2002.

**Bourg IC**, Bourg ACM, Sposito G. The surface proton chemistry of montmorillonite. 1<sup>st</sup> International Meeting on Clays in Natural and Engineered Barriers for Radioactive Waste Confinement, Reims, December 2002.

**Bourg IC**, Bourg ACM, Sposito G. Diffusion and adsorption in compacted bentonite. 8<sup>th</sup> International Conference on the Chemistry and Migration Behavior of Actinides and Fission Products in the Geosphere, Bregenz, September 2001.

## **TEACHING**

### **Courses taught**

“The Environmental Nexus,” Princeton University (2017)

“Interfacial Waters in Natural Systems,” Princeton University (2016, 2018)

“Intro to Environmental Engineering,” Princeton University (2015, 2016, 2017)

“Carbon Capture and Sequestration,” UC Berkeley (2011, 2013, 2014)

### **Undergraduate Research Advising**

#### Senior theses

2017-18 – A Byrnes, L Watt.

2016-17 – V Amaral, A Chang, S Jacobson, K Shizuru.

2015-16 – S Wang, M Williams.

#### Junior independent study

2018 – R Lussier.

#### Summer research internships

2018 – A Cavazos, SI Higashino, KN Underwood.

### **Postdoctoral Scholars Supervised (at Princeton, unless otherwise noted):**

Bastien Wild, 2018-present (co-supervised with C White).

Ayumi Koishi, 2018-present.

Thomas Underwood, 2017-present.

Greeshma Gadikota, 2016-2017 (now Assistant Professor, University of Wisconsin Madison).

Baptiste Dazas, 2015-2017 (now Assistant Professor, University of Poitiers, France).

Lauren Beckingham, 2012-2014, Earth Sciences Division, Lawrence Berkeley National Laboratory (now Assistant Professor, Auburn University; co-supervised with CI Steefel).

Michael Holmboe, 2011-2012, Earth Sciences Division, Lawrence Berkeley National Laboratory (now Assistant Professor, University of Umeå, Sweden).

### **Graduate Students Supervised, as Major Advisor:**

Jennifer AR Willemsen, 2015-present.

Emily Wei-Hsin Sun, 2016-present.

Xinyi Shen, 2016-present.

Francisco J Carrillo, 2016-present.

Mihiro Nomura, 2017-present.

Xiaohan Li, 2018-present.

### **PhD Defense Committees:**

2016 – Z Zhang.

2015 – H Deng, B Guo.

### **PhD Annual Review Committees:**

2018 – K DeCarlo, K Gong, ER McCaslin, D Ramos, MP Ruiz, A Santos, K Spokas, K Yang, J Young.

2017 – K DeCarlo, K Gong, H Hunter, MP Ruiz, AE Sherman, K Spokas, JAW Willemsen, K Yang.

2016 – K DeCarlo, F Georget, Z Zhang.

2015 – Z Zhang.

#### **PhD Qualifying Examination Committees:**

2018 – FJ Carrillo, S Hartzell, X Shen, W Shuai, EWH Sun, S Yue.

2017 – ER McCaslin, J Young, JAR Willemsen, H Hunter, A Sherman.

2016 – L Golston, K Gong, K Spokas, X He, K Yang.

2015 – MP Ruiz, K DeCarlo.

2010 – LN Nielsen (UC Berkeley).

### **PROFESSIONAL ACTIVITIES (Internal)**

#### **University Committees**

Committee on Committees (2017-present).

#### **Other Academic Service**

##### Civil and Environmental Engineering

Undergraduate Advising, Environmental Engineering track (2017-present).

Undergraduate Advising, Geological Engineering track (2016-present).

##### Princeton Environmental Institute

PEI Anniversary Committee (2017-present).

##### School of Engineering and Applied Science

Freshman Advising (2016-17).

##### Geological Engineering Program

Geological Engineering Program Executive Committee (2015-present).

### **PROFESSIONAL ACTIVITIES (External)**

#### **Service to Scientific Societies**

Member of the Committee on Council Nominations, Clay Minerals Society (2016-present).

Editor of the bi-monthly CMS News page published in the journal *Elements*, Clay Minerals Society (2013-2015).

#### **Professional Society Memberships**

American Chemical Society (ACS), Association of Environmental Engineering and Science Professors (AEESP), American Geophysical Union (AGU), Clay Minerals Society (CMS), European Association of Geochemistry (EAG), Mineralogical Society of America (MSA), Soil Science Society of America (SSSA).

#### **Manuscript Reviews for Journals**

Reviewer of 110 manuscripts for 30 scholarly journals: Accounts of Chemical Research, Acta Geotechnica, Advances in Water Resources, Applied Clay Science, Applied Geochemistry, Chemosphere, Clays and Clay Minerals, Colloids and Surfaces, Croatica Chimica Acta, Environmental Science: Processes and Impacts, Environmental Science and Technology, Geochimica et Cosmochimica Acta, Geophysical Perspectives Letters, International Journal of Greenhouse Gas Control, Journal of the American Chemical Society, Journal of Colloid and Interface Science, Journal of Contaminant Hydrology, Journal of Geophysical Research, Journal of Hydrology, Journal of Physical Chemistry, Langmuir, Molecular Physics, Nature Communications, Nuclear Technology, Physical Chemistry Chemical Physics, Proceedings of the National Academy of Sciences of the USA, Science, SPE Journal, Vadose Zone Journal, Water Resources Research.

### **Editing of Scientific Journals**

Guest Editor of a special issue of *Accounts of Chemical Research* on the Chemistry of Geologic Carbon Storage, jointly with DJ DePaolo, UC Berkeley (2017).  
Associate Editor for *Frontiers in Energy Research* (2014-present).

### **Service to Governmental Agencies**

Ad-hoc reviewer of 25 proposals for the US Department of Energy (DOE), the National Science Foundation (NSF), the French Agence Nationale de la Recherche (ANR), the US Defense Threat Reduction Agency, the Swiss NSF, the German Research Foundation (DFG), the Portuguese Science and Technology Foundation (FCT), and the Foundation for Polish Science (FPS).  
Panelist on three proposal review panels for the NSF (both in 2016) and the US DOE (2017).

### **Leadership of International Workshops and Short Courses**

Workshop on “Molecular Dynamics Simulations” at the Goldschmidt conference in Paris (2017). (Jointly with M Holmboe, LN Lammers, and K Kulasinski)  
Short course on “Geochemistry of geologic CO<sub>2</sub> sequestration” in Berkeley (2013). (Jointly with DJ DePaolo, DR Cole, and A Navrotsky under the auspices of the Mineralogical Society of America)  
Workshop on “Microscopic-scale view of CO<sub>2</sub> sequestration” at the European Center for Atomistic and Molecular Modeling (CECAM) in Lausanne (2011). (Jointly with B Rotenberg)

### **Invited Panelist/Discussion Leader at Scientific Meetings**

Invited discussion leader, Gordon Research Conference on Water and Aqueous Solutions, Holderness (2018).  
Invited session chair, International Conference on Clays in Natural and Engineered Barriers for Radioactive Waste Confinement, Davos (2017).  
Invited discussion leader, Gordon Research Conference on Carbon Capture, Utilization, and Storage, Easton (2015).  
Invited panelist, DOE Office of Science workshop on Basic Research Needs for Environmental Management, Washington (2015).

### **Leadership of Large Collaborative Research Projects**

Member of the Executive Committee and leader of one of the three Thrust Areas of the Center for Nanoscale Controls on Geologic CO<sub>2</sub>, a DOE Office of Science Energy Frontiers Research Center with ~20 co-PIs (2011-2018).

### **Organization of Conference Sessions**

Computational Methods in Water Resources (CMWR) conference (2018).  
Goldschmidt conference (2009, 2009, 2015, 2017).  
American Chemical Society (ACS) meeting (2014).  
American Geophysical Union (AGU) meeting (2008, 2010).

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