

IAN C BOURG

Civil & Environmental Engineering / High Meadows Environmental Institute
E-208 E-Quad, Princeton University, Princeton NJ 08544
ph: 609-258-4541; email: bourg@princeton.edu; web: bourg.princeton.edu

EDUCATION

BEng, Chemical Engineering, National Institute of Applied Sciences, Toulouse (1999).
MSc, Chemical Engineering, National Institute of Applied Sciences, Toulouse (1999).
PhD, Civil and Environmental Engineering, University of California, Berkeley (2004).

PROFESSIONAL POSITIONS

Assistant Professor, Department of Civil and Environmental Engineering and High Meadows Environmental Institute, Princeton University (2015-present).
Research Scientist, Earth Sciences Division, Lawrence Berkeley National Laboratory (2009-2014).
Visiting Postdoc Scholar, Department of Geophysical Sciences, University of Chicago (2008).
Postdoc Scholar, Earth Sciences Division, Lawrence Berkeley National Laboratory (2005-2009).

HONORS & AWARDS

Howard B. Wentz junior faculty award, Princeton SEAS (2020).
NSF CAREER Award, US National Science Foundation (2018).

EXTRAMURAL FUNDING (at Princeton, \$3.1M since 2015)

Department of Energy, Office of Science, Office of Basic Energy Sciences, Geosciences Program, “Nanoscale Basis of the Permeability of Fine-Grained Sedimentary Rocks,” 2021-2024; \$600,000 awarded to Bourg (PI).
National Science Foundation, Division of Chemical, Bioengineering, Environmental and Transport Systems, Environmental Engineering Program, “Adsorption of Per- and Polyfluoroalkyl Substances (PFASs) and Other Polar Organic Contaminants on Pristine and Organic-Coated Clay Mineral Surfaces,” 2019-2022; \$329,992 awarded to Bourg (PI).
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, “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; \$275,000 awarded to Bourg during 2016-2020.
Department of Energy, Office of Science, Office of Basic Energy Sciences, Energy Frontiers Research Center (EFRC) Program grant, “Center for Nanoscale Controls on Geologic CO₂ (NCGC),” 2014-2018 (director: DJ DePaolo; executive committee: IC Bourg, J Ajo-Franklin, CI Steefel); \$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 CO₂ Sequestration*, Reviews in Mineralogy and Geochemistry, Vol 77, Mineralogical Society of America (2013).

PEER-REVIEWED PUBLICATIONS (Bourg group members in bold)

Dr Bourg has published 49 peer-reviewed journal papers, book chapters, or comments (*h*-index of 28 in Scopus, 32 in Google Scholar).

Willemssen JAR, Emunah M, Bourg IC. Adsorption of organic contaminants on soil organic matter coated smectite clay particles. *Soil Science Society of America Journal*, in press (2022).

Carrillo FJ, Soulaire C, Bourg IC. The impact of sub-resolution porosity on numerical simulations of multiphase flow. *Advances in Water Resources*, 104094 (2022).

Lee SS, **Koishi A, Bourg IC**, Fenter P. Ion correlations drive charge overscreening and heterogeneous nucleation at solid-aqueous electrolyte interfaces. *Proceedings of the National Academy of Sciences* 118, e2105154188 (2021).

Carrillo FJ, Bourg IC. Capillary and viscous fracturing during drainage in porous media. *Physical Review E* 103, 063106 (2021).

Kleber M, **Bourg IC**, Coward EK, Hansel CM, Myneni SCB, Nunan N. Dynamic interactions at the mineral-organic matter interface. *Nature Reviews Earth & Environment* 2, 402-421 (2021).

Carrillo FJ, Bourg IC. Modeling multiphase flow within and around deformable porous materials: A Darcy-Brinkman-Biot approach. *Water Resources Research* 57, e2020WR028734 (2021).

Yang JQ, Zhang X, Bourg IC, Stone HA. 4D imaging reveals mechanisms of clay-carbon protection and release. *Nature Communications* 12, 622 (2021).

Lee SS, **Koishi A, Bourg IC**, Fenter P. Visualizing salinity-dependent evolution of the electrical double layer at a charged solid-water interface. *Science*, submitted (2021).

Carrillo FJ, Bourg IC. Capillary and viscous fracturing during drainage in porous media. *Physical Review E*, in review (2021).

Kleber M, **Bourg IC**, Coward E, Hansel CM, Myneni SCB, Nunan N. Mineral-organic interactions: Emerging views and new frontiers. *Nature Reviews Earth & Environment*, in review (2021).

Yang JQ, Zhang X, Bourg IC, Stone HA. 4D imaging reveals mechanisms of clay-carbon protection and release. *Nature Communications*, in press (2021).

Carrillo FJ, Bourg IC. Modeling multiphase flow within and around deformable porous materials: A Darcy-Brinkman-Biot approach. *Water Resources Research*, in press (2021).

Willemssen JAR, Bourg IC. Molecular dynamics simulation of the adsorption of per- and polyfluoroalkyl substances (PFASs) on smectite clay. *Journal of Colloid and Interface Science* 585, 337-346 (2021).

Shen X, Bourg IC. Molecular dynamics simulations of the colloidal interaction between smectite clay nanoparticles in liquid water. *Journal of Colloid and Interface Science* 584, 610-621 (2021).

Sun EWH, Bourg IC. Molecular dynamics simulation of mineral surface wettability by water versus CO₂: thin films, contact angles, and capillary pressure in a silica nanopore. *Journal of Physical Chemistry C* 124, 25382-25395 (2020).

Carrillo FJ, Bourg IC, Soulaire C. Multiphase flow modelling in multiscale porous media: An open-sourced micro-continuum approach. *Journal of Computational Physics X* 8, 100073 (2020).

Fernandez-Martinez A, Tao J, Wallace AF, **Bourg IC**, Johnson MR, De Yoreo JJ, Sposito G, Cuello GJ, Charlet L. Curvature-induced hydrophobicity at imogolite-water interfaces. *Environmental Sciences: Nano* 7, 2759-2772 (2020).

Underwood TR, Bourg IC. Large-scale molecular dynamics simulation of the dehydration of a suspension of smectite clay nanoparticles. *Journal of Physical Chemistry C* 124, 3702-3714 (2020).

- Carrillo FJ, Bourg IC.** A multi-scale computational fluid dynamics (CFD) approach for simulating flow in saturated porous media containing coarse grains, macropores, and deformable microporous clay regions. *Water Resources Research* 55, 8096-8121 (2019).
- Wild B, Daval D, Micha J-S, Bourg IC, White CE, Fernandez-Martinez A.** Physical properties of interfacial layers developed on weathered silicates: a case study based on labradorite feldspar. *Journal of Physical Chemistry C* 123, 24520-24532 (2019).
- Willemssen JAR, Myneni S, Bourg IC.** Molecular dynamics simulations of the adsorption of phthalate esters on smectite clay surfaces. *Journal of Physical Chemistry C* 123, 13624-13636 (2019).
- 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 (CO₂, CH₄, H₂, 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 CO₂ 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 ³⁶Cl⁻ 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 CO₂- and CO₃-brine-mineral systems. In: *Geochemistry of Geologic CO₂ 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 CO₂-water interfacial tension under pressure and temperature conditions of geologic CO₂ 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-CaCl₂) 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*, 2nd 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⁺ 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 or is slated to give 83 invited lectures. Additionally, to the best of his knowledge, his students, postdocs, and collaborators have given an additional 15 invited lectures on which he was listed as a co-author.

Bourg IC. *Presentation title to be determined.* Gordon Research Conference on the Chemistry and Physics of Liquids, Holderness, August 2023. (meeting delayed due to Covid-19; ICB invited by N Levinger, Colorado State U, and C Mundy, Pacific Northwest National Lab)

Carrillo FJ, Bourg IC. Biofilm hydrodynamics as a function of biofilm permeability, rheology, and fluid flow rate. AGU Fall meeting, New Orleans, December 2021.

Carrillo FJ, Bourg IC. Multiphase flow modeling in multiscale deformable porous media: An open-source micro-continuum approach. Society of Industrial and Applied Mathematics (SIAM) Conference on Mathematical & Computational Issues in the Geosciences (GS21), June 2021.

Bourg IC. Migration of water and CO₂ in clayey media. ExxonMobil, May 2021. (virtual seminar due to Covid-19; host: MD Lacasse)

Bourg IC. Clay, water, and salt: Controls on the permeability and mechanics of fine-grained sedimentary media. Marine Chemistry & Geochemistry seminar series, Woods Hole Oceanography Institute. (virtual seminar due to Covid-19; hosts: H Kim and A Dunlea)

Underwood TR, **Bourg IC.** Dielectric spectra of water in charged clay interlayer nanopores. American Chemical Society Spring meeting, April 2021. (virtual meeting due to Covid-19; ICB invited by K Yuan, Oak Ridge National Lab, A Wallace, U of Delaware, and YJ Kim, Argonne National Lab)

Willemssen JAR, **Bourg IC.** Adsorption and aggregation of soil organic matter at the clay-water interface. American Chemical Society Spring meeting, April 2021. (virtual meeting due to Covid-19; ICB invited by Y Hu, U of Houston, S Riechers and S Mergelsberg, Pacific Northwest National Lab, and M Whittaker, Lawrence Berkeley National Lab)

Wild B, White CE, **Bourg IC.** Coupled fluxes of water and ions (NaCl) during flow through silica nanopores. American Chemical Society Spring meeting, April 2021. (virtual meeting due to Covid-19; ICB invited by N Kabengi, Georgia State U, AG Ilgen, Sandia National Lab, J Loring, Pacific Northwest National Lab, and J Weber, U of Arizona)

Lee SS, Koishi A, Bourg IC, Fenter P. Salinity-dependent evolution of the electrical double layer at the muscovite (001)-water interface. American Chemical Society Spring meeting, April 2021.

Underwood TR, Shen X, Bourg IC. Molecular dynamics simulation prediction of clay swelling as a function of aqueous chemistry. American Geophysical Union Fall meeting, December 2020. (virtual meeting due to Covid-19)

Bourg IC. Clay, water, and salt: Controls on the permeability and mechanics of fine-grained sedimentary media. Seminar series of the Levich Institute, CCNY, September 2020. (virtual due to Covid-19; host: J Morris)

Bourg IC. Water on clay: Electrical double layer, disjoining pressure, and colloidal aggregation at Earth's most abundant interface. Goldschmidt conference, June 2020. (virtual meeting due to Covid-19; ICB invited by M Rildley and D Tunega). **[Keynote presentation]**

Underwood TR, Bourg IC. From atoms to aggregates: large-scale molecular dynamics simulation of the dehydration of a suspension of smectite clay nanoparticles. Clay Minerals Society (CMS) annual meeting, October 2020. (virtual meeting due to Covid-19)

Willemssen JAR, Bourg IC. Molecular dynamics simulations of the associations between smectite clay nanoparticles, soil organic matter coatings, and organic contaminants. Clay Minerals Society (CMS) annual meeting, October 2020. (virtual meeting due to Covid-19)

Wild B, White CE, Bourg IC. Multi-scale transport and textural properties of Si-rich amorphous interfacial layers. American Ceramic Society, Glass and Optical Materials Division annual meeting (GOMD 2020), August 2020. (virtual meeting due to Covid-19)

- Koishi A, Sun EW-H, Lee SS, Michot L, Fenter P, Fernandez-Martinez A, **Bourg IC**. Water uptake at the mica-water interface: from single molecules to clusters, films, and droplets. American Chemical Society Spring meeting, Philadelphia, March 2020. (conference cancelled due to Covid-19; ICB invited by J Bracco, N Kabengi, and K Yuan)
- Underwood TR, **Bourg IC**. Molecular dynamics simulation of a clay nanoparticle suspension during dehydration. American Chemical Society Spring meeting, Philadelphia, March 2020. (conference cancelled due to Covid-19; ICB invited by Y Hu, S Mergelsberg, S Riechers, M Whittaker, and M Zhu)
- Lee SS**, Koishi A, Bourg IC, Fenter P. Ion cooperativity at the muscovite (001)-brine interface. American Chemical Society Spring meeting, Philadelphia, March 2020. (conference cancelled due to Covid-19)
- Bourg IC**. Water on clay: MD simulations of charge screening, hydrophobic adsorption, and colloidal mechanics at Earth's most abundant interface. Seminar series of the Chemistry in Solution and at Interfaces (CSI) center, Princeton, February 2020. (ICB invited by R Car)
- Bourg IC**. Coupled hydrology, chemistry, and mechanics of clay-rich sedimentary rocks: from molecular to meter scales. Annual technical meeting of the Society of Engineering Science, Washington University, St. Louis, October 2019. (ICB invited by LR Pestana, U of Miami)
- Bourg IC**. Clay, water, and salt: Controls on the hydrology of fine-grained sedimentary rocks. Department of Civil and Environmental Engineering, Northwestern University, October 2019. (host: L Aristilde)
- Bourg IC**. Clay, water, and salt: Controls on the permeability and mechanics of fine-grained porous media. Department of Geosciences, Georgia State University, October 2019. (host: N Kabengi)
- Bourg IC**, Carrillo FJ, Shen X, Underwood TU. Clay, water, and salt: Controls on the permeability of fine-grained sedimentary rocks. Goldschmidt conference, Barcelona, August 2019. (ICB invited by C Chen, Dalian U Technol). **[Keynote presentation]**
- Bourg IC**. Clay, water, and salt: Controls on the hydrology of fine-grained sedimentary rocks. Department of Geosciences, University of Oslo, June 2019. (host: F Renard)
- Bourg IC**. Mineral-organic interactions in soils and sediments. Swedish Chemical Society annual meeting, Umeå, June 2019. (ICB invited by JF Boily and M Holmboe, U of Umeå)
- Bourg IC**. Hydro-chemo-mechanical coupling in fine-grained soils and sedimentary rocks. Department of Civil and Environmental Engineering, UC Irvine, May 2019. (host: MJ Abdolhosseini Qomi)
- Bourg IC**. Liquid water at interfaces. Division of Materials Science, Physical and Computational Sciences, Pacific Northwest National Lab, May 2019. (hosts: J De Yoreo and K Rosso)
- Bourg IC**. Clay, water, and salt: Controls on the hydrology of fine-grained soils and sedimentary rocks. PHENIX Laboratory, University of Paris-Sorbonne/CNRS, April 2019. (host: V Marry)
- Koishi A**, Lee SS, Fenter P, Fernandez-Martinez A, Michot L, Bourg IC. Surface hydrophobicity and energetics at mica-water interfaces. American Chemical Society Spring meeting, Orlando, April 2019.
- Bourg IC**. Clay, water, and salt: Controls on the hydrology of fine-grained soils and sedimentary rocks. Department of Civil and Environmental Engineering, New Jersey Institute of Technology, April 2019. (host: J Meegoda)
- Bourg IC**. Clay, water, and salt: Controls on the hydrology of fine-grained soils and sedimentary rocks. Department of Earth and Environmental Science, Temple University, March 2019. (host: IV Buynevich)
- Bourg IC**. Clay, water, and salt: Controls on the hydrology of fine-grained soils and sedimentary rocks. Department of Earth, Atmospheric, and Planetary Sciences, Purdue University, January 2019. (host: LJ Pyrak-Nolte)

- Bourg IC.** Molecular basis of soil carbon protection by mineral surfaces. Soil Science Society of American annual meeting, San Diego, January 2019. (ICB invited by OW Duckworth, NC State University)
- Bourg IC.** Clay, water, and salt: Controls on the hydrology of fine-grained soils and sedimentary rocks. Department of Civil, Environmental, and Ocean Engineering, Stevens Institute of Technology, October 2018. (host: V Prigiobbe)
- 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 (CO₂, CH₄, 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⁺ 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⁺ 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⁺ 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), 32nd 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), 32nd 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 Newey, 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 CO₂ 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. 5th 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 CO₂ sequestration. Department of Civil and Environmental Engineering, University of Connecticut, September 2012. (host: A MacKay)
- Bourg IC.** Nanoscale basis of CO₂-brine multiphase flow and geochemistry in CO₂ storage repositories. Center for Frontiers of Subsurface Energy Security (CFSES), Sandia National Laboratories, June 2012. (host: R Cygan)
- Bourg IC.** Nanoscale basis of CO₂-brine multiphase flow and geochemistry in CO₂ 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 CO₂-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 CO₂: 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)

- Willemsen JAR, **Bourg IC.** Adsorption of phthalate esters and perfluorinated alkyl substances (PFAS) on organic-coated smectite clay. AGU Fall meeting, New Orleans, December 2021.
- Sun EWH, **Bourg IC.** Molecular dynamics simulations of silica wettability by water versus CO₂ in the presence of organic matter. AGU Fall meeting, New Orleans, December 2021.
- Agles A,** Bourg IC. Replica exchange molecular dynamics (REMD) simulations to uncover the molecular architecture of the biofilm matrix. AGU Fall meeting, New Orleans, December 2021.
- Carrillo FJ,** Bourg IC. Simulation and machine learning prediction of clogging processes in porous media. AGU Fall meeting, New Orleans, December 2021.
- Li X,** Bourg IC. Molecular dynamics simulations of liquid water microphysics in nano-aerosol droplets. AGU Fall meeting, New Orleans, December 2021.
- Shen X,** Bourg IC. Coarse-grained simulation prediction of microstructure and mechanics in clay-water mixtures. AGU Fall meeting, New Orleans, December 2021.
- Yang JQ,** Zhang X, Bourg IC, Stone H. 4D imaging reveals mechanisms of clay-carbon protection and release. AGU Fall meeting, New Orleans, December 2021.

- Reina CA**, Wild B, Cama J, Bourg IC. Mineral weathering and nutrient cycling at the early stages of soil development. Goldschmidt conference, July 2021. (virtual meeting due to Covid-19)
- Shen X**, Bourg IC. Coarse-grained simulation of chemo-mechanical coupling in swelling clay. Goldschmidt conference, July 2021. (virtual meeting due to Covid-19)
- Sun EWH**, Bourg IC. Molecular dynamics simulations of mineral surface wettability in the presence of carbon dioxide and organics. Goldschmidt conference, July 2021. (virtual meeting due to Covid-19)
- Wild B**, White CE, Bourg IC. Molecular dynamics simulation of water and ion permeation across silica nanopores in the context of silicate weathering. Goldschmidt conference, July 2021. (virtual meeting due to Covid-19)
- Zhariyeva Z**, Fernandez-Martinez A, Van Driessche A, Cuello G, Claret F, Bourg IC. The structure of water in calcium-silicate-hydrates studied by neutron diffraction with isotopic substitution. ERICA-CASH II conference, Heidelberg, January 2021. (virtual meeting due to Covid-19)
- Carrillo FJ**, Bourg IC. Multiphase flow modelling in multiscale deformable porous media: An open-sources micro-continuum approach. Computational Methods in Water Resources (CMWR) conference, December 2020. (virtual meeting due to Covid-19)
- Shen X**, Bourg IC. Free energy of aggregation of charged colloids (smectite clay) in liquid water from molecular dynamics simulations. Clay Minerals Society (CMS) annual meeting, Richland, October 2020. (virtual meeting due to Covid-19)
- Yang JQ**, Zhang X, Bourg IC, Stone HA. 4D imaging reveals mechanisms of clay-carbon protection and release. Clay Minerals Society (CMS) annual meeting, October 2020. (virtual meeting due to Covid-19)
- Carrillo FJ**, Bourg IC. Multiphase flow modelling in multiscale deformable porous media: An open-sources micro-continuum approach. AGU Fall meeting, December 2020. (virtual meeting due to Covid-19)
- Bourg IC**. Interaction of organic molecules with smectite clay minerals: A review. Goldschmidt conference, June 2020. (virtual meeting due to Covid-19)
- Shen X**, Bourg IC. Free energy of aggregation of charged colloids (smectite clay) in liquid water from molecular dynamics simulations. Goldschmidt conference, June 2020. (virtual meeting due to Covid-19)
- Sun EWH**, Bourg IC. Wettability of mineral surfaces by water and carbon dioxide. Goldschmidt conference, June 2020. (virtual meeting due to Covid-19)
- Underwood TR**, Bourg IC. Molecular dynamics simulations of diffusion in the clay matrix. Goldschmidt conference, June 2020. (virtual meeting due to Covid-19)
- Wild B**, White CE, Bourg IC. Multiscale investigation of fluid-silicate interfaces and their control on dissolution kinetics. Goldschmidt conference, June 2020. (virtual meeting due to Covid-19)
- Willemsen JAR**, Bourg IC. Metadynamics based molecular dynamics simulation of the adsorption of per- and polyfluoroalkyl substances on smectite clay surfaces. Goldschmidt conference, June 2020. (virtual meeting due to Covid-19)
- Yang JQ**, Bourg IC, Zhang X, Stone H. 4D imaging of clay reveals soil carbon dynamics. Goldschmidt conference, June 2020. (virtual meeting due to Covid-19)
- Soulaine C**, Carrillo FJ, Bourg IC. A (real) multi-scale solver for two-phase flow: a micro-continuum approach. Interpore conference, Qingdao, May 2020. (conference cancelled due to Covid-19)
- Shen X**, Bourg IC. Free energy of interaction of two smectite clay nanoparticles in liquid water. American Chemical Society Spring meeting, Philadelphia, March 2020. (conference cancelled due to Covid-19)
- Underwood TR**, Coward E, Ohno T, Sparks DL, Bourg IC. Molecular simulations of soil organic matter at the goethite-water interface. American Chemical Society Spring meeting, Philadelphia, March 2020. (conference cancelled due to Covid-19)

- Wild B**, White CE, Bourg IC. Control of the macroscopic dissolution rates of silicate materials by nanoporous interfacial layers. American Chemical Society Spring meeting, Philadelphia, March 2020. (conference cancelled due to Covid-19)
- Willemsen JAR**, Bourg IC. Molecular dynamics simulation of the adsorption of per- and polyfluoroalkyl substances on smectite clay surfaces. American Chemical Society Spring meeting, Philadelphia, March 2020. (conference cancelled due to Covid-19)
- Li X**, Bourg IC. How secondary organic aerosol affects precipitation and radiative forcing. AGU Fall meeting, San Francisco, December 2019.
- Lee SS**, Bracco JN, Bourg IC, Stack AG, Fenter P. Hydration structure at mineral-water interfaces. American Chemical Society Fall meeting, San Diego, August 2019.
- Koishi A**, Lee SS, Fenter P, Fernandez-Martinez A, Michot LJ, Sun EWH, Bourg IC. Surface hydrophobicity and energetics at mica-water interfaces. Goldschmidt conference, Barcelona, August 2019.
- Shen X**, Bourg IC. Free energy of interaction of two smectite clay nanoparticles in liquid water. Goldschmidt conference, Barcelona, August 2019.
- Sun EWH**, Bourg IC. Molecular dynamics simulation of mica wetting by water and organics. Goldschmidt conference, Barcelona, August 2019.
- Underwood TR**, Bourg IC. Molecular dynamics simulations of nanoconfined water in the clay matrix. Goldschmidt conference, Barcelona, August 2019.
- Wild B**, Koishi A, Fernandez-Martinez A, Daval D, White CE, Bourg IC. Control of silicate-fluid interactions by nanoporous interfacial systems. Goldschmidt conference, Barcelona, August 2019.
- Willemsen JAR**, Bourg IC. Metadynamics based molecular dynamics simulation and experimental study of the adsorption of per- and polyfluoroalkyl substances on smectite clay surfaces. Goldschmidt conference, Barcelona, August 2019.
- Bourg IC**. Mineral-organic interactions in soils and sediments. US DOE, Office of Basic Energy Sciences, Geosciences Program PI meeting, Washington DC, August 2019.
- Bourg IC**, Carrillo FJ, Shen X, Underwood T. Coupled hydrology, chemistry, and mechanics of fine-grained soils and sedimentary rocks. Euroclay 2019 quadrennial meeting, Paris, July 2019.
- Fernandez-Martinez A**, Wallace AF, Tao J, Bourg IC, Johnson MR, Cuello GJ, Charlet L. Curvature-induced hydrophobicity at imogolite-water interfaces: ‘The nanotube effect’. Euroclay 2019 quadrennial meeting, Paris, July 2019.
- Koishi A**, Lee SS, Fenter P, Fernandez-Martinez A, Michot L, Bourg IC. Surface hydrophobicity and energetics at mica-water interfaces. Euroclay 2019 quadrennial meeting, Paris, July 2019.
- Shen X**, Bourg IC. Free energy of interaction of two smectite clay nanoparticles in liquid water. Euroclay 2019 quadrennial meeting, Paris, July 2019.
- Underwood TR**, Bourg IC. Properties of clay-rich fine-grained sedimentary rocks from large scale molecular dynamics simulations. Euroclay 2019 quadrennial meeting, Paris, July 2019.
- Willemsen JAR**, Myneni S, Bourg IC. Adsorption of phthalate esters on smectite clay surfaces: A molecular dynamics simulation and experimental study. Euroclay 2019 quadrennial meeting, Paris, July 2019.
- Bourg IC**, Carrillo FJ, Shen X, Underwood TR. Chemo-mechanical coupling in fine-grained soils and sedimentary rocks. European Association of Geoscientists and Engineers shale workshop, Bordeaux, April 2019.
- Nomura M**, Bourg IC. Molecular dynamics simulations of semi-volatile organic aerosol particles containing water, black carbon, and α -pinene secondary organic compounds. European Geosciences Union general assembly, Vienna, April 2019.
- Carrillo FJ**, Bourg IC. A multiphase Darcy-Brinkman-Biot approach towards modeling hydrology and mechanics of deformable porous media: model derivation and application to fine-grained and fractured porous media. Interpore Conference, Valencia, May 2019.

- Bourg IC.** Clay, water, and salt: Controls on the permeability of fine-grained sedimentary rocks. Workshop on Transport in Disordered Environments, Princeton Center for Theoretical Studies, Princeton, January 2019.
- Bourg IC.** Clay, water, and salt: Controls on the permeability of fine-grained sedimentary rocks. American Geophysical Union fall meeting, Washington DC, December 2018.
- Carrillo FJ, Bourg IC.** A multi-scale computational fluid dynamics approach for simulating multi-phase flow in deformable porous media. American Geophysical Union fall meeting, Washington DC, December 2018.
- Nomura M, Bourg IC.** Molecular dynamics (MD) simulations of black carbon and α -pinene secondary organic aerosol at the air-water interface. American Geophysical Union fall meeting, Washington DC, December 2018.
- Shen X, Bourg IC.** Free energy of interaction of two smectite clay nanoparticles in liquid water. American Geophysical Union fall meeting, Washington DC, December 2018.
- Sun EWH, Bourg IC.** Molecular dynamics simulation prediction of quartz wetting by water and supercritical CO₂ and the potential impact of organic residues. American Geophysical Union fall meeting, Washington DC, December 2018.
- Underwood TR, Bourg IC.** Transport properties of clay-rich fine-grained sedimentary rocks from large scale molecular dynamics simulations. American Geophysical Union fall meeting, Washington DC, December 2018.
- Wild B, White CE, Bourg IC.** Impact of pore-scale processes on silicate dissolution kinetics. American Geophysical Union fall meeting, Washington DC, December 2018.
- Willemssen J, Myneni S, Bourg IC.** Molecular dynamics simulation and experimental study of the adsorption of phthalate esters on smectite clay surfaces. American Geophysical Union fall meeting, Washington DC, December 2018.
- Bourg IC.** HCM coupling in fine-grained sedimentary media. Symposium on Energy Geotechnics, Lausanne, September 2018.
- 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 CO₂. 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.
- Willemssen 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.
- Dazas 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 CO₂. 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. 7th 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.
- Willemsen 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 (CO₂, CH₄, H₂, 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 (CH₄, CO₂, H₂, 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⁺ 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**, Beekingham 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 CaCl₂ electrolyte: a molecular dynamics study. 6th 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 CO₂- and CO₃-brine-mineral systems. Mineralogical Society of American short course on the Geochemistry of Geologic CO₂ Sequestration, Berkeley, December 2013.
- Liu Y, **Bourg IC**. Wettability of silica by brine vs. CO₂: 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. CO₂: The nanoscale view. EFRC PI meeting, US Department of Energy, Washington DC, July 2013.
- Bourg IC**. Geochemistry and seal integrity in GCS. 12th 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 D₂O 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. EFRC 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 CO₂-brine interface: predicting geologic CO₂ storage capacities and characteristics. Goldschmidt conference, Knoxville, June 2010.
- Bourg IC,** Sposito G. Ion exchange selectivity of smectites in the ternary system Na⁺-Ca²⁺-CaCl₂. 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. 12th 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⁺ and Sr²⁺ tracers in compacted, saturated Na-bentonite. 10th 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. 2nd 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. 1st 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. 8th 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, 2019, 2021)
“Interfacial Waters in Natural Systems,” Princeton University (2016, 2018, 2021)
“Intro to Environmental Engineering,” Princeton University (2015, 2016, 2017, 2018, 2019, 2020, 2021)
“Carbon Capture and Sequestration,” UC Berkeley (2011, 2013, 2014)

Undergraduate Research Advising

Senior theses

2021-22 – C Adkins, K Contreras-Godfried, E Cruz, M McHugh, R Mohamed, CC Wayner.
2020-21 – M Emunah, J Giguere, C Reina.
2019-20 – SI Higashino, KN Underwood
2018-19 – A Cavazos, R Lussier, C Nwatchukwu.
2017-18 – A Byrnes, L Watt.
2016-17 – V Amaral, A Chang, S Jacobson, K Shizuru.
2015-16 – S Wang, M Williams.

Independent study

2021-22 – A Lemay, N Martin, R Neapole, E Sontarp.
2020-21 – A Gourabathina, N Ralston.
2019-20 – R Mohamed.
2018-19 – KN Underwood.
2017-18 – R Lussier.

Summer research internships

2021 – JP Alvarado, D Gonzalez, A Lemay, R Neapole, E Sontarp, M Wiese.
2020 – A Celik, S Cho, G Dickinson, A Gourabathina, B Henry, Y Iwasaki, P Maruri, R Mohamed, N Ralston, CA Reina.
2018 – A Cavazos, SI Higashino, KN Underwood.

Postdoctoral Scholars Supervised (at Princeton, unless otherwise noted)

Xiaojin Zheng, 2021-present.
Bastien Wild, 2018-present (co-supervised with CE White).
Thomas R Underwood, 2017-present.
Ayumi Koishi, 2018-2020. (now Postdoc Scholar, Lawrence Berkeley National Lab)
Greeshma Gadikota, 2016-2017 (now Assistant Professor, Cornell University).
Baptiste Dazas, 2015-2017 (now Assistant Professor, University of Poitiers, France).
Lauren Beckingham, 2012-2014, Lawrence Berkeley National Lab (now Assistant Professor, Auburn University).
Michael Holmboe, 2011-2012, Lawrence Berkeley National Lab (now Associate Professor, University of Umeå, Sweden).

Graduate Students Supervised, as Major Advisor (PhD unless noted otherwise)

Xiaohan Li, 2018-present.
Avery Agles, 2018-present.
Mihiro Nomura, 2017-2019 (MSE).
Xinyi Shen, 2016-present.
Emily Wei-Hsin Sun, 2016-present.
Francisco J Carrillo, 2016-2021.

Jennifer AR Willemsen, 2015-2021 (now Scientist at the New Jersey Department of Environmental Protection).

PhD Defense Committees (Princeton CEE, unless noted otherwise)

2021 – FJ Carrillo (Princeton CBE), W Shuai, JAR Willemsen, S Yue (Princeton CBE).

2020 – S Hartzell, H Hunter, AE Sherman, K Yang, J Young (Princeton CBE).

2019 – S Calabrese, K DeCarlo, L Golston, K Gong, D Ramos (Princeton Geosciences), V Ramothe (U of Paris), M Ruiz, A Santos (Princeton CBE), K Spokas.

2016 – Z Zhang.

2015 – H Deng, B Guo.

MSE Defense Committees (Princeton CEE, unless noted otherwise)

2019 – M Nomura.

PhD Annual Review Committees (Princeton CEE, unless noted otherwise)

2020-21 – A Agles, K Alventosa, M Curria, J Duan (Princeton Geosciences), X Li, ER McCaslin (Princeton CBE), M Muniz (Princeton CBE), T Postma, X Shen, EWH Sun, J Schneider (Princeton CBE), J Weis (Princeton CBE).

2019-20 – K Alventosa, J Duan (Princeton Geosciences), ER McCaslin (Princeton CBE), T Postma, X Shen, AE Sherman, EWH Sun, JAR Willemsen, S Yue (Princeton CBE).

2018-19 – FJ Carrillo (Princeton CBE), K DeCarlo, J Duan (Princeton Geosciences), K Gong, S Hartzell, ER McCaslin (Princeton CBE), D Ramos (Princeton Geosciences), X Shen, AE Sherman, K Spokas, EWH Sun, JAR Willemsen, K Yang, J Young (Princeton CBE), S Yue (Princeton CBE).

2017-18 – K DeCarlo, K Gong, H Hunter, ER McCaslin (Princeton CBE), D Ramos (Princeton Geosciences), MP Ruiz, A Santos (Princeton CBE), AE Sherman, K Spokas, JAR Willemsen, K Yang, J Young (Princeton CBE).

2016-17 – K DeCarlo, K Gong, MP Ruiz, K Spokas, K Yang.

2015-16 – K DeCarlo, F Georget, Z Zhang.

2014-15 – Z Zhang.

PhD Qualifying Examination Committees (Princeton CEE, unless noted otherwise)

2021 – C Geissler (Princeton CBE).

2020 – SK Anand, Z Bajalan, M Curria, J Duan (Princeton Geosciences), X Li, M Muniz (Princeton CBE), C Pu, J Schneider (Princeton CBE), J Weis (Princeton CBE).

2019 – K Alventosa, J Kim, N Li (twice), T Postma.

2018 – FJ Carrillo (Princeton CBE), S Hartzell, X Shen, W Shuai, EWH Sun, S Yue (Princeton CBE).

2017 – ER McCaslin (Princeton CBE), J Young (Princeton CBE), 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

Director of Undergraduate Studies, Acting (Fall 2021).

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

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

High Meadows Environmental Institute

HMEI Director of Graduate Studies (2019-present).

Walbridge Fund Graduate Award committee leader (2019-present).

School of Engineering and Applied Science

Freshman Advising (2016-17, 2019-20).

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), American Society of Civil Engineers (ASCE), 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 136 manuscripts for 37 scholarly journals: *Accounts of Chemical Research*, *ACS Earth and Space Chemistry*, *Acta Geotechnica*, *Advances in Water Resources*, *Applied Clay Science*, *Applied Geochemistry*, *Chemical Reviews*, *Chemosphere*, *Clays and Clay Minerals*, *Colloids and Surfaces*, *Croatica Chimica Acta*, *Environmental Science: Nano*, *Environmental Science: Processes and Impacts*, *Environmental Science and Technology*, *Fluid Phase Equilibria*, *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*, *Journal of Physical Chemistry Letters*, *Langmuir*, *Molecular Physics*, *Nano Letters*, *Nature Communications*, *Nuclear Technology*, *Physical Chemistry Chemical Physics*, *Proceedings of the National Academy of Sciences*, *Science*, *Soil Science Society of America Journal*, *SPE Journal*, *Vadose Zone Journal*, and *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* (2014-2019).

Service to Governmental Agencies

Ad-hoc reviewer of 44 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 National Science Foundation, the German Research Foundation (DFG), the Portuguese Science and Technology Foundation (FCT), the Foundation for Polish Science (FPS), the American Chemical Society Petroleum Research Fund (ACS PRF), and the Swiss National Supercomputing Center.

Panelist on nine proposal review panels for the NSF [2016 ($\times 2$), 2019, 2020 ($\times 3$), 2021] and the US DOE (2017, 2020).

Leadership of International Workshops and Short Courses

Workshop on “Physics in the Ground Beneath our Feet” at the Princeton Center for Theoretical Studies (2022). (Jointly with S Datta, CY Lai, and HA Stone)

Workshop on “Transport in Disordered Environments” at the Princeton Center for Theoretical Studies (2019). (Jointly with S Datta and A Kosmrlj)

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 CO₂ 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 CO₂ 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 CO₂, 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).

American Chemical Society (ACS) meeting (2014).

Goldschmidt conference (2009, 2009, 2015, 2017, 2020).

American Geophysical Union (AGU) meeting (2008, 2010).

January 31, 2022