

## IAN C BOURG

Civil & Environmental Engineering / High Meadows Environmental Institute  
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### 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

Associate Professor, Department of Civil and Environmental Engineering and High Meadows Environmental Institute, Princeton University (2022-present).  
Visiting Professor, Department of Civil, Environmental, and Geomatic Engineering, Swiss Federal Polytechnic Institute (ETH), Zurich (2022-2023).  
Assistant Professor, Department of Civil and Environmental Engineering and High Meadows Environmental Institute, Princeton University (2015-2022).  
Research Scientist (career-track), Earth Sciences Division, Lawrence Berkeley National Laboratory (2009-2014).  
Postdoctoral 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).

### 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

Dr Bourg has published 56 peer-reviewed journal papers, book chapters, or comment (*h*-index of 31 in Scopus, 35 in Google Scholar). An additional 2 papers are currently under review.

Agles A, Bourg IC. Structure-thermodynamic relationship of a polysaccharide gel (alginate) as a function of water content and counterion type (Na vs. Ca). *Journal of Physical Chemistry B*, in review (2022).

Li X, Bourg IC. Microphysics of liquid water in sub-10 nm ultrafine aerosol particles. *Atmospheric Chemistry and Physics*, in review (2022).

Shen X, Bourg IC. Interaction between hydrated smectite clay particles as a function of salinity (0 to 1 M) and counterion type (Na, K, Ca). *Journal of Physical Chemistry C*, in press (2022).

Calabrese S, Wild B, Bertagni MB, Bourg IC, White CE, Abruto F, Cipolla G, Noto LV, Porporato A. Nano-to global-scale uncertainties in terrestrial enhanced weathering. *Environmental Science and Technology*, in press (2022).

Sun EWH, Bourg IC. Impact of organic solutes on capillary phenomena in water-CO<sub>2</sub>-quartz systems. *Journal of Colloid and Interface Science* 629A, 265-275 (2023).

- Koishi A, Lee SS, Fenter P, Fernandez-Martinez A, Bourg IC. Water adsorption on mica surfaces with hydrophilicity tuned by counterion type (Na, K, Cs) and structural fluorination. *Journal of Physical Chemistry C* 126, 16447-16460 (2022).
- Zhakiyeva Z, Cuello GJ, Fischer HE, Bowron DT, Dejoie C, Magnin V, Campillo S, Bureau S, Poulain A, Besselink R, Gaboreau S, Grangeon S, Claret F, Bourg IC, Van Driessche AES, Fernandez-Martinez A. Structure of water adsorbed on nanocrystalline calcium silicate hydrate determined from neutron scattering and molecular dynamics simulations. *Journal of Physical Chemistry C* 126, 12820-12835 (2022).
- Kurz DL, Secchi E, Carrillo FJ, Bourg IC, Stocker R, Jimenez-Martinez J. Competition between growth and shear stress drives intermittency in preferential flow paths in porous media biofilms. *Proceedings of the National Academy of Sciences* 119, e2122202119 (2022).
- Wild B, White CE, Bourg IC. Molecular dynamics simulations of reverse osmosis in silica nanopores. *Journal of Physical Chemistry C* 126, 9161-9172 (2022).
- Underwood TR, Bourg IC. Dielectric properties of water in charged nanopores. *Journal of Physical Chemistry B* 126, 2688-2698 (2022).
- Willemsen JAR, Emunah M, Bourg IC. Adsorption of organic contaminants on soil organic matter coated smectite clay particles. *Soil Science Society of America Journal* 86, 238-252 (2022).
- Carrillo FJ, Soullaine 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).
- Willemsen 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 simulations of mineral surface wettability by water versus CO<sub>2</sub>: thin films, contact angles, and capillary pressure in a silica nanopore. *Journal of Physical Chemistry C* 124, 25382-25395 (2020).
- Carrillo FJ, Bourg IC, Soullaine C. Multiphase flow modeling in multiscale porous media: An open-source 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 Darcy-Brinkman-Biot approach to modeling the hydrology and mechanics of porous media containing macropores and deformable microporous 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).
- Willemsen JAR, Myneni SCB, 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 KM, 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).
- 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. Stern layer structure and energetics 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, Dufrêche 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 LE, 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. 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, Schäfer 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, Larson TE, 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* 109, 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 liquid 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 sodium 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).

## PROFESSIONAL ACTIVITIES

### 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 139 manuscripts for 37 scholarly journals, primarily *Environmental Science and Technology*, *Geochimica et Cosmochimica Acta*, and the *Journal of Physical Chemistry*.

### **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 CO<sub>2</sub> sequestration” in Berkeley under the auspices of the Mineralogical Society of America (2013). (Jointly with DJ DePaolo, DR Cole, and A Navrotsky)

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)

### **Organization of Conference Sessions**

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

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

Computational Methods in Water Resources (CMWR) conference (2018).

American Chemical Society (ACS) meeting (2014).

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