

## IAN C BOURG

Assistant Professor, tenure-track

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## EDUCATION

**National Institute of Applied Sciences, Toulouse.** Chemical Engineering, BEng, 1999.

**National Institute of Applied Sciences, Toulouse.** Chemical Engineering, MSc, 1999.

**University of California, Berkeley.** Civil and Environmental Engineering, PhD, 2004.

## APPOINTMENTS

**2015-** **Assistant Professor**, Civil and Environmental Engineering, Princeton University

**2009-2014** **Research Scientist**, Earth Sciences, Lawrence Berkeley National Laboratory.

**2008** **Visiting Postdoctoral Fellow**, Geophysical Sciences, University of Chicago.

**2005-2009** **Postdoctoral Fellow**, Earth Sciences, Lawrence Berkeley National Laboratory.

## 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 PAPERS AND BOOK CHAPTERS

Lammers LN, **Bourg IC**, Okumura M, Kolluri K, Sposito G, Machida M. Molecular dynamics simulations of cesium adsorption on illite nanoparticles. *J. Colloid Interface Sci.*, in press.

Tournassat C, Davis JA, Chiaberge C, Grangeon C, **Bourg IC**. Modeling the acid-base properties of montmorillonite edge surfaces. *Environ. Sci. Technol.*, in press.

Tournassat C, **Bourg IC**, Holmboe M, Sposito G, Steefel CI. Molecular dynamics simulations of anion exclusion in clay interlayer nanopores. *Clays Clay Miner.* 64:374-388.

Tinnacher RM, Holmboe M, Tournassat C, **Bourg IC**, Davis JA. Ion adsorption and diffusion in smectite: molecular, pore, and continuum scale views. *Geochim. Cosmochim. Acta*, 177:130-149 (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. *Appl. Clay Sci.* 123:18-28 (2016).

**Bourg IC**. Sealing shales versus brittle shales: A sharp threshold in the material properties and energy technology uses of fine-grained sedimentary rocks. *Environ. Sci. Technol. Letters* 2:255-259 (2015).

**Bourg IC**, Beckingham L, DePaolo DJ. The nanoscale basis of CO<sub>2</sub> trapping for geologic storage. *Environ. Sci. Technol.* 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, Schäfer T. Complete restriction of  $^{36}\text{Cl}^-$  diffusion by celestite precipitation in densely compacted illite. *Environ. Sci. Technol. Lett.* 2:139-143 (2015).
- 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. *Chem. Geol.* 372:119-143 (2014).
- Holmboe M, **Bourg IC**. Molecular dynamics simulations of water and sodium diffusion in smectite interlayer nanopores as a function of pore size and temperature. *J. Phys. Chem. C* 118:1001-1013 (2014).
- Hamm LM, **Bourg IC**, Wallace AF, Rotenberg B. Molecular simulation of  $\text{CO}_2^-$  and  $\text{CO}_3^-$ -brine-mineral systems. In: *Geochemistry of Geologic  $\text{CO}_2$  Sequestration* (DJ DePaolo, DR Cole, A Navrotsky, & IC Bourg, eds.), Reviews in Mineralogy and Geochemistry, Vol. 77, pp. 189-228, Mineralogical Society of America (2013).
- Hofmann AE, **Bourg IC**, DePaolo DJ. Ion desolvation as a mechanism for kinetic isotope fractionation in aqueous systems. *Proc. Natl. Acad. Sci. U.S.A.*, 198:18689-18694 (2012).
- Nielsen LC, **Bourg IC**, Sposito G. Predicting  $\text{CO}_2$ -water interfacial tension under pressure and temperature conditions of geologic  $\text{CO}_2$  storage. *Geochim. Cosmochim. Acta* 81:28-38 (2012).
- Bourg IC**, Steefel CI. Molecular dynamics simulations of water structure and diffusion in silica nanopores. *J. Phys. Chem. C* 116:11556-11564 (2012).
- Bourg IC**, Sposito G. Molecular dynamics simulations of the electrical double layer on smectite surfaces contacting concentrated mixed electrolyte ( $\text{NaCl-CaCl}_2$ ) solutions. *J. Colloid Interface Sci.* 360:701-715 (2011).
- Bourg IC**, Sposito G. Ion exchange phenomena. In: *Handbook of Soil Science, 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 to the continuum scale for diffusion processes in smectite-rich porous media. *Environ. Sci. Technol.* 44:2085-2091 (2010).
- Bourg IC**, Richter FM, Christensen JN, Sposito G. Isotopic mass-dependence of metal cation diffusion coefficients in liquid water. *Geochim. Cosmochim. Acta* 74:2249-2256 (2010).
- 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, & TW Lyons. *Geochim. Cosmochim. Acta* 72:5852-5854 (2008).
- Bourg IC**, Sposito G, Bourg ACM. Modeling the diffusion of  $\text{Na}^+$  in compacted water-saturated Na-bentonite as a function of pore water ionic strength. *Appl. Geochem.* 23:3635-3641 (2008).
- Bourg IC**, Sposito G. Isotopic fractionation of noble gases by diffusion in liquid water: Molecular dynamics simulations and hydrologic applications. *Geochim. Cosmochim. Acta* 72:2237-2247 (2008).
- Bourg IC**, Sposito G, Bourg ACM. Modeling the acid-base surface chemistry of montmorillonite. *J. Colloid Interface Sci.* 312:297-310 (2007).
- Bourg IC**, Sposito G, Bourg ACM. Modeling cation diffusion in compacted water-saturated sodium bentonite at low ionic strength. *Environ. Sci. Technol.* 41:8118-8122 (2007).
- Bourg IC**, Sposito G. Molecular dynamics simulations of kinetic isotope fractionation during the diffusion of ionic species in liquid water. *Geochim. Cosmochim. Acta* 71:5583-5589 (2007).
- Bourg IC**, Sposito G, Bourg ACM. Tracer diffusion in compacted, water-saturated bentonite. *Clays Clay Miner.* 54:363-374 (2006).
- Bourg IC**, Bourg ACM, Sposito G. Modeling diffusion and adsorption in compacted bentonite: a critical review. *J. Contam. Hydrol.* 61:293-302 (2003).

Jakobsen HA, **Bourg I**, Hjarbo KW, Svendsen HF. Interaction between reaction kinetics and flow structure in bubble column reactors. In: *Parallel Computational Fluid Dynamics – Trends and Applications*, Elsevier, 543-550 (2001).

## TEACHING EXPERIENCE

### Lecturer

*Interfacial Waters in Natural Systems*, Princeton University (2016).

*Intro to Environmental Engineering*, Princeton University (2015, 2016).

*Carbon Capture and Sequestration*, University of California, Berkeley (2011, 2013, 2014).

### Guest Lecturer

*Advection, diffusion, and adsorption in natural and engineered clay barriers*, guest lecture for *Special Topics in Environmental Aspects of Nuclear Engineering* (Instructors: J Ahn and J Birkholzer), University of California, Berkeley (2014)

*Simulation de l'eau dans les matériaux nanoporeux*, guest lecture to 4<sup>th</sup> and 5<sup>th</sup> year students in Process and Environmental Engineering at the National Institute of Applied Sciences (INSA), Toulouse (2012).

*Clays, Ions, and Water: the Molecular-Scale View*, guest lecture for a short course on *Application of Molecular Simulations to Oil and Gas Industry* (Instructor: Y Liang), Kyoto University (2011).

*Molecular Dynamics Simulations of the Clay-Water Electric Double Layer*, guest lecture for *Surface and Colloid Chemistry of Natural Particles* (Instructor: G Sposito), University of California, Berkeley (2010).

### Graduate Student Instructor

*Water Chemistry* (Instructor: SW Hermanowicz), University of California, Berkeley (2003).

*Environmental Engineering* (Instructors: WW Nazaroff, WJ Riley), University of California, Berkeley (2002, 2003).

## HONORS & AWARDS

Winner, US DOE Life at the Frontiers of Energy Research Video Competition, for the video *Carbon in Underland* (2011).

Doctoral Fellowships (Joseph Dias fellowship, Eugene Henry fellowship), Environmental Engineering Group, UC Berkeley (2000, 2002).

“Pass with honors”, Comprehensive Examination, Environmental Engineering graduate program, UC Berkeley (2001).

Doctoral Fellowship, French Agency for the Management of Radioactive Waste (ANDRA) (1999-2002).

Leonardo Scholarship for research abroad, European Union (1999).

## SERVICE AND OUTREACH

### Organization of international workshops and short courses

*Geochemistry of geologic CO<sub>2</sub> sequestration*. Mineralogical Society of America (MSA) short course organized in Berkeley. Co-conveners: DJ DePaolo, DR Cole, A Navrotsky (2013).

*Microscopic-scale view of CO<sub>2</sub> sequestration*. Workshop organized with support from the European Center for Atomistic and Molecular Modeling (CECAM) in Lausanne, Switzerland. Co-convenor: B Rotenberg (2011).

### Organization of conference sessions

*Goldschmidt conference* (2009, 2009, 2015).

*ACS meeting* (2014).

AGU meeting (2008, 2010).

### **Reviewing**

Reviewer of 95 manuscripts for *Geochimica et Cosmochimica Acta* (28), *Environmental Science and Technology* (20), and other journals.

Ad-hoc reviewer of 19 proposals for the US DOE (6), the NSF (6), the French Agence Nationale de la Recherche (ANR) (2), 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).

Participant on two review committees for the NSF Environmental Engineering program.

### **Participation in scientific panels**

*Gordon conference on Carbon Capture, Utilization, and Storage (CCUS)*: session chair (2015).

*Basic Research Needs for Environmental Management* workshop of the DOE Office of Science: panelist (2015).

### **Editorial work**

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

### **Academic committees**

Doctoral dissertation qualifying examination committee at UC Berkeley: LN Nielsen (2010).

Doctoral dissertation qualifying examination (general examination) committees at Princeton University: M Ruiz (2015), K DeCarlo (2015), L Golston (2016), K Gong (2016), K Spokas (2016), X He (2016), K Yang (2016).

Doctoral dissertation defense committees at Princeton University: H Deng (2015), B Guo (2015).

## **INVITED PRESENTATIONS**

### **Plenary keynote presentation**

2012 – 5<sup>th</sup> International Meeting on Clays in Natural and Engineered Barriers for Radioactive Waste Confinement (Montpellier, France).

### **Invited talks at conferences, symposia, workshops, and seminars**

2016 – 10 invited talks: ACS meeting (San Diego); CMS meeting (Atlanta); Goldschmidt conference (Yokohama); ACS meeting (Philadelphia – two talks); Geodynamics seminar series (Lamont-Doherty Earth Observatory); Geosciences seminar series (U Delaware); EPS and EECE seminar series (Washington University in St Louis); Pierce seminar series (MIT).

2015 – 6 invited talks: ACS meeting (Denver – two talks); Goldschmidt conference (Prague – one invited talk, one keynote talk); DOE EFRC PI meeting (Washington DC); AGU meeting (San Francisco).

2014 – 8 invited talks: Center for Isotope Geochemistry seminar series (UC Berkeley); CMS meeting (College Station, TX – two talks); workshop on the Characterization of Nanoporous Materials (Stanford U); Molecular Foundry users' meeting (LBNL); Réunion des Sciences de la Terre (Pau); SKB Task Force meeting (Berkeley – two talks).

2013 – 1 invited talk: ACS meeting (New Orleans).

2012 – 7 invited talks: International Seminar Series on Environmental Radioactivity (Hokkaido University); APS workshop on Metal Ion Adsorption at Interfaces (Argonne National Laboratory); 2012 Young Engineers & Scientists Symposium (Berkeley); Environmental Engineering seminar series (University of Connecticut); Geology seminar series (University of Illinois at Urbana-

Champaign); Geophysical Laboratory seminar series (Carnegie Institute in Washington, DC); Center for Frontiers of Subsurface Energy Security (CFSES) seminar series (Sandia National Laboratory).

2011 – 5 invited talks: Symposium on Application of Nano-geosciences in Petroleum Engineering (Kyoto University); Goldschmidt conference (Prague); EFRC Summit and Forum (Washington DC); LBNL Advisory Board meeting (LBNL); Energy and Environmental Systems Seminar Series (Hokkaido University).

2010 – 4 invited talks: DOE workshop on the Chemistry of Novel Isotope Effects in the Geosciences (San Francisco); Seismology Lab seminar series (UC Berkeley); Center for Isotope Geochemistry seminar series (UC Berkeley); Ecosystem Sciences seminar series (UC Berkeley).

2009 – 1 invited talk: ACS meeting (Salt Lake City).

2007 – 3 invited talks: DOE Workshop on Molecular Dynamics and Structure of Geofluids (Berkeley); European Union workshop on Surface Reactions & Electrical Interfacial Layer (Opatjia, Croatia); Workshop on Environment, Neutrons and Molecular Dynamics (U of Grenoble).

2005 – 2 invited talks: International Workshop on Waste Management (Hokkaido U); International Clay Conference (Tokyo).

## RESEARCH SUPPORT

### Research Grants

2014-2018: US Department of Energy, Office of Basic Energy Sciences (DOE-BES) funding for the *Center for Nanoscale Control of Geologic CO<sub>2</sub>*, an Energy Frontiers Research Center.

2014-2017: US Department of Energy, Office of Basic Energy Sciences (DOE-BES) funding for *The Effect of Salinity of Geochemical Processes in Confined Aqueous Fluids*.

2014-2017: Japanese Atomic Energy Agency (JAEA) funding for *Repository Geoscience and PA Technology Development*.

### Allocations of supercomputer time

2015: US Department of Energy, National Energy Research Scientific Computing Center (NERSC) allocation of 10 M processor hours.

## PROFESSIONAL ASSOCIATIONS

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