Thomas R Underwood

Education

2013–2017 **PhD Earth Sciences**, *Durham University*, Durham - UK,
Graduation Date: Jan 2018
Thesis Title: Molecular Simulations of Low-Salinity Enhanced Oil Recovery
Advisors: Prof. H. Chris Greenwell, Dr. Pablo Cubillas, Dr. Valentina Erastova

2009–2013 **MPhys Theoretical Physics**, *The University of York*, York - UK, *1st Class Honours.*
Thesis Title: The Theory of Colloid Stability
Advisor: Dr. Martin Smalley

Research Appointments

2017–Present **Postdoctoral Fellow**, *Princeton University*, Princeton, NJ, USA,
Department of Civil and Environmental Engineering
Advisor: Ian C. Bourg.
Successful research goals include:
- Modeling the dielectric properties of water at the mineral-liquid interface.
- Understanding flow and transport of water and ions through clay-rich media.
- Calculating the physics underlying kinetic and equilibrium isotope fractionation in water.

2013–2017 **Graduate Researcher**, *Durham University*, Durham - UK,
Department of Earth Sciences
Advisor: H. Chris Greenwell. PhD thesis title: *Molecular Simulations of Low-Salinity Enhanced Oil Recovery (EOR)*.
Successful research goals include:
- Computational chemistry simulations of mineral-organic interactions as a function of salinity.
- Parameter analysis for the simulation of water-vapour and water-oil interfacial tension.
- Understanding contact angle variations as a function of salinity through mean-field theories and computational chemistry simulations.

References

Ian C. Bourg
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Princeton, NJ, 08544.

H. Chris Greenwell
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Durham, DH1 3LE, UK.

Valentina Erastova
Frequent collaborator
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Joseph Black Building
University of Edinburgh
Edinburgh, EH9 3FJ, UK.

Additional references available upon request.

Publications

[1] Agles A, **Underwood TR**, and Bourg IC. Water dynamics in the biofilm matrix: the dielectric properties of biofilm water. *In preparation*.

[2] Xiaojin Z, **Underwood TR**, and Bourg IC. Ion diffusion dynamics in geologically relevant fine-grained sedimentary phases: A large-scale molecular dynamics study. *In preparation*.

[3] **Underwood TR** and Bourg IC. Understanding the mystery of mass-dependent kinetic isotope fractionation. *In preparation*.

[4] **Underwood TR** and Bourg IC. Dielectric properties of water in charged nanopores. *The Journal of Physical Chemistry B*, 2022.

[5] **Underwood TR** and Bourg IC. Large-scale molecular dynamics simulation of the dehydration of a suspension of smectite clay nanoparticles. *The Journal of Physical Chemistry C*, 124(6):3702–3714, 2020.

[6] **Underwood TR** and Greenwell HC. The water-alkane interface at various nacl salt concentrations: a molecular dynamics study of the readily available force fields. *Scientific reports*, 8(1):1–11, 2018.

[7] Tian S, Erastova V, Lu S, Greenwell HC, **Underwood TR**, Xue H, Zeng F, Chen G, Wu C, and Zhao R. Understanding model crude oil component interactions on kaolinite silicate and aluminol surfaces: toward improved understanding of shale oil recovery. *Energy & Fuels*, 32(2):1155–1165, 2018.

[8] **Underwood TR**, Erastova V, and Greenwell HC. Ion adsorption at clay-mineral surfaces: the hofmeister series for hydrated smectite minerals. *Clays and Clay Minerals*, 64(4):472–487, 2016.

[9] **Underwood TR**, Erastova V, and Greenwell HC. Wetting effects and molecular adsorption at hydrated kaolinite clay mineral surfaces. *The Journal of Physical Chemistry C*, 120(21):11433–11449, 2016.

[10] **Underwood TR**, Erastova V, Cubillas P, and Greenwell HC. Molecular dynamic simulations of montmorillonite–organic interactions under varying salinity: an insight into enhanced oil recovery. *The Journal of Physical Chemistry C*, 119(13):7282–7294, 2015.

Grants and Awards

January 2017	Durham University Research Grant	
		Travel and subsistence costs for a 4 week visit to Prof. H. Heinz at CU Boulder
May 2016	The Clay Minerals Society Student Poster Award	*1st place*
May 2016	The Clay Minerals Society Student Oral Paper Award	*2nd place*
March 2016	The Clay Minerals Society Blair Jones/Jane Flynn Award	*Best student abstract*
March 2016	The Clay Minerals Society Student Travel Award	
		Travel grant to attend the meeting of the CMS, Atlanta, GA, 2016
Dec. 2015	Durham Energy Institute Small Research Grant	
		Travel and subsistence costs for a 6 week visit Prof. P. Coveney at UCL
May 2015	Department of Earth Sciences, DU, Presentation Award	
		Best 2nd year graduate student presentation
March 2015	The Mineralogical Society Travel Award	*Travel subsidy for Euroclay 2015, Edinburgh*
March 2015	Ustinov College Travel Award	*Travel subsidy for Thermodynamics 2015, Copenhagen*
October 2015	Centre of Doctoral Training in Energy PhD Research Grant	
		Additional 6 months' tuition and stipend for graduate studies

Invited Talks

May 2021 **Underwood TR**. Dielectric spectra of water in charged clay interlayer nanopores. *Sandia National Labs Department of Geochemistry seminar series*. Host: J. A. Greathouse.

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

October 2020 **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 (virtual meeting due to Covid-19)*.

August 2019 **Underwood TR**. Lecture series for Molecular Simulations of Minerals and Materials. *The University of Maine, Orono, Maine*. Host: T. Ohno.

July 2017 **Underwood TR**, Erastova V, Greenwell HC. AIPEA School for Young Scientist: Thermodynamic Analysis of MD Simulation. *AIPEA International Clay Conference, Granada, Spain*.

May 2017 **Underwood TR**, Greenwell HC. Understanding Wettability Alterations at the Molecular Scale. *CECAM workshop on Atomistic Simulations in Cementitious Systems, Les Diablerets*.

January 2017 **Underwood TR**, Erastova V, Greenwell HC. Enhancing Oil Recovery; Molecular Dynamic Simulations of Low–Salinity Enhanced Oil Recovery. *Department of Chemical and Biological Engineering, University of Colorado Boulder*. Host: H. Heinz.

Select Conference Presentations

June 2020 **Underwood TR**, Bourg IC. Molecular dynamics simulations of diffusion in the clay matrix. *Goldschmidt conference. (virtual meeting due to Covid-19)*.

March 2020 **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 (conference cancelled due to Covid-19)*.

August 2019 **Underwood TR**, Bourg IC. Molecular dynamics simulations of nanoconfined water in the clay matrix. *Goldschmidt conference, Barcelona*.

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 **Underwood TR,** Boek E, Greenwell HC. Salinity Induced Wettability Alterations – A Molecular Dynamics Study. *Euroclay 2019 quadrennial meeting, Paris*.

Dec. 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*.

August 2018 **Underwood TR**, Bourg IC. Emergent properties of clay: Molecular dynamics simulations of nanoconfined water in the clay matrix. *Goldschmidt conference, Boston*.

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 **Underwood TR**, Bourg IC. Properties of fine-grained clay-rich sedimentary rocks. *Gordon Research Conference on Flow and Transport in Permeable Media, Newry*.

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*.

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*.

July 2017 **Underwood TR,**, Greenwell HC. Understanding Wettability Alterations at the Molecular Scale. *AIPEA International Clay Conference (ICC), Granada, Spain*.

June 2016 **Underwood TR,** Erastova V, Greenwell HC. MD Simulations of Low-Salinity Enhanced Oil Recovery. *Meeting of the Clay Mineral Society (CMS), Atlanta*.

May 2016 **Underwood TR,** Erastova V, Greenwell HC. Enhancing Oil Recovery: Molecular Dynamic Simulations of Low–Salinity Enhanced Oil Recovery. *Meeting of the Clay Mineral Society (CMS), Atlanta*.

Sep. 2015 **Underwood TR,** Erastova V, Greenwell HC. Enhancing Oil Recovery - Using Free Energy Calculations to Help Explain Low-Salinity Enhanced Oil Recovery. *Thermodynamics 2015, Copenhagen*.

July 2015 **Underwood TR,** Erastova V, Greenwell HC. Enhancing Oil Recovery: Molecular Dynamic Simulations of Low–Salinity Enhanced Oil Recovery. *Euroclay 2015 quadrennial meeting, Edinburgh*.

June 2015 **Underwood TR,** Erastova V, Greenwell HC. Molecular Simulations of Low–Salinity Enhanced Oil Recovery. *CECAM: Atomistic simulations in Earth Sciences, Paris*.

Professional Activities

Professional Society Affiliations

American Chemical Society (ACS); American Geophysical Union (AGU); Geochemical Society; the Clay Minerals Society (CMS).

Peer-Review for Academic Journals

Reviewer of over 20 manuscripts for 13 academic journals: ACS Applied Materials & Interfaces; ACS Applied Nano Materials; ACS Energy & Fuels; ACS Journal of Physical Chemistry; ACS Langmuir; Applied Clay Science; Chemical Physics Letters; Clays and Clay Minerals; European Journal of Soil Science; Journal of Colloid and Interface Science; Journal of Hydrology; Journal of Petroleum Science and Engineering; International Journal for Numerical and Analytical Methods in Geomechanics.

Conference Organising Sessions

I am currently helping to convene a session on "Clays and Computational Science" at the upcoming AIPEA XVII International Clay Conference / Meeting of the Clay Minerals Society in summer 2022.

Teaching and Mentoring Experience

Classes taught include:

- Intro to Environmental Engineering. Princeton University. Precepts and office hours.
- Introductory Mathematics for Earth Scientists. Durham University.
- Matlab for Geosciences. Durham University.
- Physics and Mathematics for Chemistry. Durham University.
- Physical Chemistry Labs II. Durham University.

I have mentored several students at various points of their academic career to date:

- Postdoctoral researchers: Xiaojin Zheng.
- PhD students: Avery Agles, Shansi Tian.
- Master's thesis students: Lucas Powell-Rudden, Kevin Kendaru, Joshua Tasker, Jess Leung, Leon Devereux.
- Undergraduate summer students: K. Nye Underwood.