



DEPARTMENT OF ENVIRONMENTAL SCIENCES

Presents a Seminar by:

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“Modelling Dynamics in Solids: From Origin of Life to Modern Challenges”

FRIDAY, FEBRUARY 28, 2020

1:00PM

Room 223

Environmental & Natural Resource Sciences Bldg.
14 College Farm Road, New Brunswick, NJ

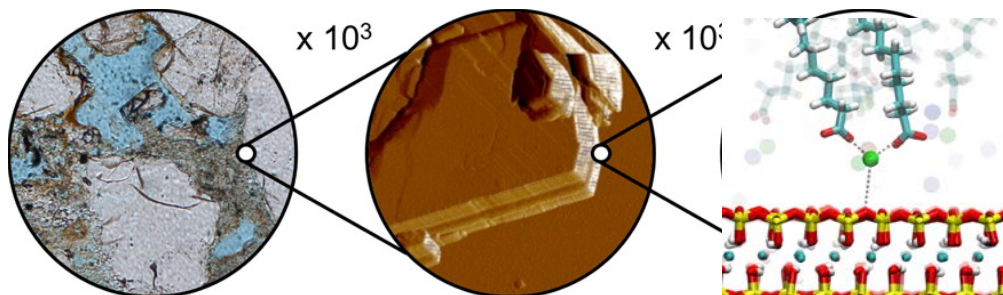
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Environmental Sciences Seminars- <http://envsci.rutgers.edu/seminars.html>

Abstract:

- What interactions are key for retaining carbon in soils?
- Why some solvents are better at creating “high-surface” materials?
- How pollutants can be captured and retained by layered minerals?
- What is the role of minerals in the Origin of Life?

These seemingly unrelated questions share a common feature – they rely on specific physicochemical interactions between small molecules and soil-forming minerals.

Molecular modelling is a powerful tool allowing us to rationalise existing data and produce testable hypotheses. Within this talk, on examples from my work [1-6], I will demonstrate how computational techniques allow us to obtain atomistic information on large-scale processes occurring on our planet and beyond. I intend this talk to be an introduction to molecular modelling of minerals, and to promote fruitful interdisciplinary conversations.



Electron scanning microscope image (left) of a sandstone core, atomic force microscope image (centre), and atomistic molecular model of a montmorillonite clay interaction with organic molecule via Ca^{2+} cation bridging (right).

- [1] V Erastova, MT Degiacomi, DG Fraser & HC Greenwell, "Mineral Surface Chemistry Control for Origin of Prebiotic Peptides", *Nature Communications*, 2017
- [2] K Ruengkajorn, V Erastova, JC Buffet, HC Greenwell & D O'Hare, "Aqueous Immiscible Layered Double Hydroxides: Synthesis, Characterisation and Molecular Dynamics Simulation", *ChemComm*, 2018
- [3] T Underwood, V Erastova & HC Greenwell, "Wetting Effects and Molecular Adsorption at Hydrated Kaolinite Clay Mineral Surfaces", *The Journal of Physical Chemistry C*, 2016
- [4] B Grégoire, V Erastova, DL Geatches, SJ Clark, HC Greenwell & DG Fraser, "Insights into the Behaviour of Biomolecules on the Early Earth: The Concentration of Aspartate by Layered Double Hydroxide Minerals", *Geochimica et Cosmochimica Acta*, 2016
- [5] S Tian, V Erastova, S Lu, HC Greenwell, T Underwood, H Xue, F Zeng, G Chen & C Wu, "Understanding model crude oil component interactions at kaolinite silicate and aluminol surfaces: towards improved shale oil recovery", *Energy and Fuels*, 2017
- [6] T Underwood, V Erastova & HC Greenwell, "Ion adsorption at clay-mineral surfaces: the Hofmeister series for hydrated smectite minerals" *Clays and Clay Minerals*, 2016

Keywords: *molecular modeling, interfaces, adsorption, layered minerals, clays, origin of life*

Bio:

Valentina graduated with the undergraduate degree in chemistry from Durham University (UK). After her Master's research in theoretical chemistry at Santiago-de-Compostela (Spain), she won ORSAS scholarship to fund her PhD back at Durham University.

Valentina's research lays across material chemistry and geosciences, focusing on the study of molecular phenomena at solid interfaces. In 2018 she has been awarded Founder's Prize by British Magnetic Resonance Group for her development of molecular modelling techniques for solid-state NMR. In 2019 she received Chancellor's Fellowship at the University of Edinburgh, allowing her to start her research group.