

Department of Chemistry Seminar Series – Fall 2020

Atomistic Simulations of Smectite Hydration Processes

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Host: Prof. Cherie Yebstrebky

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Meeting Room: <https://ucf.zoom.us/j/8378887486> Passcode: 555634



Molecular modelling techniques (electronic or classical DFT, ab initio and classical molecular dynamics simulations and Monte Carlo) have emerged as useful tools to obtain detailed insights into either the structure, thermodynamics and dynamics of hydrated layered minerals and other geochemical systems [1]. Recent years development in this area has expanded the types of properties as well as range of both time and spatial scales that can be examined. These computational techniques are particularly powerful when complementing experimental techniques (spectroscopic, wet-chemical, calorimetric, scattering or diffraction techniques), hence combined experimental and *in silico* (i.e. computer simulations) investigations are steadily becoming more and more popular.

In this work, we present our most recent research efforts from molecular dynamics (MD) simulations using the Gromacs suite of programs and the Matlab ATOM scripts [2-3], along with the relevant forcefields for smectite clay minerals. The specific aim of this study was to complement experimental XRD data on smectite clay hydration and microstructure, by predicting the hydration energetics of the Wyoming type Montmorillonite for a wide range of water contents (up to 60 w% H₂O) and interlayer solutes (Li⁺, Na⁺, K⁺, Cs⁺, Ca²⁺, Mg²⁺, Cu²⁺, Cl⁻). We obtained several dynamical, thermodynamical and structural properties at different water loadings, for instance ion/water/clay atom coordination environments and residence times, hydrogen bonding behavior, diffusion coefficients, as well as immersion energies, potential of mean force (PMF) profiles and swelling pressure during Montmorillonite hydration. Furthermore, we scrutinize the main driving forces behind clay hydration, by decomposing the overall hydration energy in terms of: long-range and short-range interactions, electrostatic and VdW interactions, as well molecular component specific interactions.

[1] Cygan, R.T., Greathouse, J.A., Heinz, H., Kalinichev, A.G., *J. Mater. Chem.*, 19, 2470–2481 (2009).

[2] Abraham, M.; Van der Spoel, D.; Lindahl, E.; Hess, B., *SoftwareX*, 312, 19-25 (2014).

[3] Holmboe, M. *Clays Clay Miner.* 67, 419–426 (2019).

Bio

Michael Holmboe was born in northern Sweden in 1978 and has a MSc and PhD in Chemistry from KTH in Stockholm, Sweden. His PhD thesis focused on clay geochemistry in the context of the planned Swedish repository for high-level nuclear waste. He conducted postdoctoral research first at LBNL, Berkeley, and later at Uppsala University, Sweden, before joining the Chemistry department at Umeå university (UMU) in northern Sweden as an assistant professor in 2015. Currently he holds a permanent associate professor position at the Chemistry department/UMU, where his groups research is focused on experimental and theoretical molecular-scale characterization of layered minerals and other nanomaterials.