Postdoc: Molecular simulation of cationic exchange in clay

Supervisor: L. Brochard (Navier Laboratory, in Champs-sur-Marne, east of Paris, France)

Swelling clays are well known for their strong sensibility to hydration. Water molecules can adsorb in-between nanometric mineral layers, which causes a 'crystalline swelling' of very large local magnitude (tens of percent). Humidity, temperature and mechanical loading are all affecting water adsorption, which leads to peculiar THM couplings such as drying shrinkage[1], thermal compaction[2], and accelerated creep rate[3]. Mitigating the crystalline swelling would be of great interest for a variety of applications from geo-mechanics (e.g., confinement of geological storage), to construction (e.g., foundations on swelling soils) and infrastructures (e.g., stability of levees/dikes/dams). A way to control and mitigate crystalline swelling consists in performing cationic exchange, i.e., changing the nature of the cations in-between clay layers. The goal of this postdoc will be to use molecular simulation techniques to better understand the effects of cationic exchange in clay.

This postdoc is part of the ALLUVIUM project (I-site FUTURE) dedicated to earthen construction, with particular emphasis on the preservation of cultural heritage and the formulation of earthen materials for low carbon constructions (bricks, mortar, 3D printing). In the context of this project, an on-going experimental campaign using XRD identified a shortlist of promising cationic compounds to mitigate crystalline swelling. Yet, this identification mostly proceeds by trial and error and the reason why some compounds perform better than others remains unclear. A fine understanding of the effects of cationic exchange requires a detailed investigation at a scale hardly accessible to experiment. In this postdoc, we propose to use molecular simulation techniques to complement experiments at the nano-scale. One can fully characterize the mechanical effect of cationic exchange by evaluating how swelling free energy evolves with relative humidity and cationic composition[4]. Of particular interest will be the set of compounds identified experimentally, for which XRD data offers a direct confrontation between molecular simulations and experiments. The structure and evolution of the molecular systems will be investigated in detail to identify the reason explaining the mitigation of swelling, which could help guiding the search of efficient cationic compounds.

This postdoc offer is a one-year position. It will be hosted in Navier Laboratory, located at the Ecole Nationale des Ponts et Chaussées in Champs-sur-Marne (east of Paris, France). The position can start anytime but not later than fall 2020. The gross salary is about 2500€ per month. Applicants must hold a PhD degree in condensed matter physics, (geo)-mechanics, or related areas with a competitive track record. They must be capable to communicate in good English, including the oral and written presentation of research papers. A solid background in mechanics and physics of materials with a strong taste for numerical modeling are recommended. Expertise in the thermodynamics of clay and previous experience in molecular simulation are appreciated. Interested applicants should contact L. Brochard (laurent.brochard@enpc.fr) and provide a CV and a motivation letter.

[1] Carrier et al. (2013). Langmuir, 29(41), 12823–12833. http://doi.org/10.1021/la402781p
[2] Brochard et al. (2017). Acta Geotechnica, 12(6), 1261–1279. http://doi.org/10.1007/s11440-017-0596-3
[3] Carrier et al. (2016). Langmuir, 32(5), 1370–1379. http://doi.org/10.1021/acs.langmuir.5b03431
[4] Honorio et al. (2017). Langmuir, 33(44), 12766–12776. http://doi.org/10.1021/acs.langmuir.7b03198

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