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## Modelling realistic clay systems with ClayCode



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Clay minerals play important roles in environmental remediation, waste containment, agriculture, and pharmaceutical formulations. Their physicochemical behaviour is strongly linked to their molecular structure, and even small structural perturbations can significantly influence their performance. Molecular modelling techniques can provide atomistic insights into these systems and help interpret experimental observations. However, many molecular dynamics studies rely on oversimplified clay structures, limiting the representativeness and predictive power of computational models.

We present ClayCode [1], a Python package developed to facilitate the modelling of clay systems that closely match their experimental counterparts. It generates realistic clay structures parameterised with the ClayFF force field [2], together with input files compatible with the GROMACS simulation engine [3]. We demonstrated the utility of ClayCode in a benchmarking study of competitive barium and sodium adsorption relevant to nuclear waste disposal, as well as in a large-scale adsorption screening investigating amino acid selectivities on Martian analogue clays in astrobiological contexts. Our results emphasise the need for more accurate clay models in classical molecular dynamics simulations and show that ClayCode can be used to produce a wide variety of atomistic clay models.

[1] H. Pollak, M. Degiacomi, V. Erastova, *J. Chem. Theory Comput.*, 20, 9606-9617 (2024)

[2] R. Cygan, J. Liang, A. Kalinichev, *J. Phys. Chem. B*, 108, 1255-1266 (2004)

[3] H. Berendsen, D. van der Spoel, R. van Drunen, *Comput. Phys. Commun.*, 91, 43-56 (1995)

### **Short Bio**

Hannah Pollak has recently joined the High Performance Computing in Molecular Modelling group at LAQV as a postdoctoral researcher. In this seminar she will present her doctoral work on molecular modelling of clay minerals carried out at the School of Chemistry of the University of Edinburgh under the supervision of Valentina Erastova.

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### **Webinar Host**

António Ribeiro, High Performance Computing in Molecular Modelling Research Group