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Application of Monte Carlo Approaches to Mineral Interfaces

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One of the important goals of atomistic simulation is to reliably predict the structure, adsorption and transport at mineral surfaces. Furthermore, the interfaces are complicated by being polycrystalline rather than perfect infinite solids, and the composition at the interface is rarely the same as that of the stoichiometric bulk. Thus there is a need to develop and apply computational tools that are able to investigate the role of interface composition on interfacial and adsorption free energies. One such tool is Monte Carlo (MC).

Therefore, in this presentation we describe our recent work where we are developing and applying the MC simulation code, DL_MONTE, to help improve our modelling of complex interfaces at the atomic-level. In addition to briefly introducing the approach, we will discuss three examples. These include: lattice switch MC for evaluating surface free energies, that allow for the inclusion of explicit anharmonicity, semi-grand MC to investigate the structure and stability as a function of dopant concentrations and grand canonical MC for modelling molecular adsorption and calculating free energies as a function of distance and composition.