Ab initio molecular dynamics simulations of the water feldspar interface

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Feldspars are the most common rock-forming minerals in Earth’s crust. They are also readily found in our atmosphere in the form of dust particles. Due to their ubiquity, feldspars are of big interest to the geological and atmospheric science community. Especially the feldspar - water interface is of particular importance. Processes such as rock weathering [1] and ice nucleation in the atmosphere [2] crucially depend on the physical and chemical details of that interface. We here investigate the interface between feldspar and water to understand how water interacts with it on an atomistic length scale. To do so we use ab-initio molecular dynamics simulations. A careful analysis of the reactivity of water molecules with different chemical entities on the surface allows us to compare our ab-initio results with classical approaches such as the ClayFF forcefield and coarse grained models. The different approaches enable us to get far reaching insight, which we put into context with experimental findings concerning the reactivity of feldspar in aqueous conditions.