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Ab Initio Molecular Dynamics Simulation of Model Smectite Clay System

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After an introduction assessing the performance of Density Functional Theory (DFT) for aqueous systems we discuss the first results of an ab initio molecular dynamics (Car-Parrinello) simulation of a model smectite clay. Our system, $NaSi_{15}Al_9O_{40}(OH)_8$, is a downsized version of the classical molecular dynamics montmorillonite model of Ref. [1]. We investigate the dry clay and a system hydrated by 16 water molecules. Structure and dynamics are compared at a temperature of 300 K. The geometry of the mineral layer is found to be well preserved under hydration, while the water layer is still fairly mobile. The same holds for the sodium ion, which even in absence of solvation is not stationary on the pico second time scale of the simulation. Also the vibrational spectrum is discussed. We conclude with an outlook for the application of Car-Parrinello to this type of geochemical system.

Boek ES, Coveney PV, & Skipper NT, *J. Am. Chem. Soc.*, **117**, 12608, (1995).