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Evolution of the interlayer space of hydrated montmorillonite as a function of temperature

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Abstract

The evolution of the interlayer space of different hydrated, Wyoming-type montmorillonite under the influence of temperature was investigated by means of Monte Carlo molecular modeling simulation methods. Calculations were performed on montmorillonite with monovalent and divalent counterions including Li^+, Na^+, K^+, Rb^+, Cs^+, Ca^{2+}, Ni^{2+}, Zn^{2+}, and Pb^{2+}. For each of these clays we have conducted a series of 16 simulations in which the temperature is increased systematically from 300 to 400 K, then decreased to 260 K, and finally increased to 300 K. SPC/E water model is used to describe the water and hydroxyl behavior. From these simulations we found that the variation in the interlayer spacing of 3-layer hydrated montmorillonite is much greater than that of 2- and 1-layer hydrated montmorillonite. Hysteresis phenomena have been found in the interlayer spacing-temperature curves, especially at high temperature. The influence of temperature on the swelling behaviors of montmorillonite is different in that it depends on the counterions contained in the clay.

Keywords: Montmorillonite clay, Molecular dynamics, interlayer space, light and heavy cations