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Confined water in tunnel nanopores of sepiolite: Insights from molecular simulations

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Abstract

Sepiolite is a type of magnesium-rich fibrous clay mineral. The unique fibrous structure endows it with various applications in many fields. Revealing the behavior of confined water in sepiolite nanopores is crucial to understand the macroscopic properties of sepiolite. Aiming to ascertain the distribution and dynamics of the confined water, molecular simulations using grand canonical Monte Carlo and molecular dynamics methods have been performed. We obtain the water adsorption isotherm, density distribution profiles, and dynamic information of the confined waters in sepiolite tunnels. We find that zeolitic water is very hard to be desorbed from sepiolite under ambient conditions. Based on the distribution profile and trajectories of the water, we reveal the accurate distribution sites and propose a new distribution model of the confined water including one bound water site and four zeolitic water sites, which are determined by sepiolite lattice. The zeolitic water at different sites can exchange freely and frequently, and thus these sites may be energetically similar. This model provides more fundamental understanding of the hydration of sepiolite, and highlights the water behaviors in the tunnel pores of microporous minerals, which are thought being controlled by the crystallographic structure. The much lower mobility of zeolitic water in sepiolite than that in montmorillonite implies that materials with nano-sized tunnel pores could have more efficient fixation on foreign molecules or ions in environmental applications than those layered materials with slit pores.

Keywords: Sepiolite, zeolitic water, adsorption isotherm, molecular dynamics, grand canonical Monte Carlo