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Effects of crystal chemistry on adsorption, occurrence, and mobility of water in palygorskite tunnels

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Abstract

Palygorskite is a fibrous magnesium-rich clay mineral with a typical tunnel structure, and its adsorption properties make it an ideal adsorbent for broad applications. Thus, revealing the confinement effects on tunnel species can help in understanding its adsorption properties. Grand canonical Monte Carlo and molecular dynamics simulations were performed to analyze the effects of the crystal chemistry of palygorskite on the adsorption, occurrence, and mobility of tunnel water. Water adsorption isotherm, distribution models, and mobility were achieved from these simulations. Zeolitic water emerges into the tunnels even at a low relative humidity (RH) (such as 5%) and completely fills the tunnels as the RH increases to 10%. In neutral palygorskite, the influence of the octahedral type on water adsorption is not obvious, but the influence of tunnel cations is obvious. The occupation of Na^+ ions in tunnels can reduce the maximum water amount and affect the spatial distribution of zeolitic water. The water distribution in tunnels can be described by a two-zeolitic water-site model for neutral palygorskite and a one-zeolitic water-site model for the charged one. The zeolitic water confined in the tunnel presents very low mobility, and the appearance of Na^+ ions in the charged palygorskite further reduces the mobility of zeolitic water. Compared with other clay minerals, the much lower water mobility of palygorskite implies that it may have a more efficient fixation on foreign molecules or ions in environmental applications.

Keywords: Palygorskite, water, adsorption, molecular dynamics simulations, Grand canonical Monte Carlo, confining effects, mobility