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Molecular dynamics insight into the cointercalation of hexadecyltrimethyl-ammonium and acetate ions into smectites

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Abstract

Classical molecular dynamic simulations are performed to investigate the microscopic properties of hexadecyltrimethylammonium (HDTMA) intercalated smectites with and without the cointercalation of acetate groups. Three model smectites with distinct layer-charge characteristics are selected as the frameworks and their HDTMA intercalates correspond to the representative monolayer, bilayer, and paraffin configurations of the aliphatic chains. In the organoclays without cointercalation, all trimethyl-ammonium headgroups of HDTMA are fixed firmly above the center of the surface six-member rings through electrostatic attractions with surface oxygen, whereas the alkyl chains are a little more mobile. It is found that the cointercalations can significantly increase the basal spacings of the pure HDTMA intercalated smectites. The distributions and mobility of the HDTMA headgroups are not affected by the acetate ions because of the overwhelming attractions coming from the clay sheets. The acetate groups are fixed by the HDTMA headgroups through ion pairing. This simulation study provides a molecular level basis to understand the effects of cointercalation on properties of organoclays.

Keywords: HDTMA, acetate, molecular dynamic, smectite, cointercalation