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First-principle study of polytype structures of 1:1 dioctahedral phyllosilicates

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ABSTRACT

The polytype structures of the three 1:1 dioctahedral phyllosilicates found in nature, kaolinite, dickite, and nacrite, have been investigated, using first-principle calculations within density functional theory. The crystal structures were calculated by being optimized with relaxation of all atomic positions. The calculated structural parameters, including the orientation of the OH groups, for the three polytypes are in good agreement with experimental data. In particular, for kaolinite and dickite, the three-inner surface OH groups were predicted to be oriented nearly perpendicular to the (001) plane. In contrast, one of the inner surface OH groups of nacrite was predicted to be nearly parallel with respect to the (001) plane. Based on a comparison of formation energies, the chiral polymorphs of kaolinite (B- or C-site vacancy) have similar formation energies as dickite and nacrite, while achiral kaolinite with A-site vacancy is only slightly less stable than the other polytypes.