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All-atom ab initio energy minimization of the kaolinite crystal structure

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Abstract

Calculations that minimize the energy and optimize the geometry of all atomic coordinates for two proposed kaolinite crystal structures were performed using a first-principles, quantum chemical code based on local density functional theory. All calculations were performed using published unit-cell parameters. Inner- and interlayer H atom positions agree well with those determined by Bish (1993) from neutron diffraction data and confirm a unit cell with *C*1 symmetry.