American Mineralogist, Volume 99, pages 1962–1972, 2014

Ab initio investigations of dioctahedral interlayer-deficient mica: Modeling particles of illite found within gas shale

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Abstract

The focus of the study presented here is the illite component of the clay mineral components found within gas shale, specifically the creation of robust, atomistic models of illite particles bearing characteristics of the $2M_1$ polytype. The template for the illite models is derived from crystallographic data, which is used together with the general formula, $K_{1.67}(Al_{3.29}Fe_{0.38}Mg_{0.32})[(Si_{6.68}Al_{1.32})O_{20}(OH)_4]$ to create different particles of illite, each containing potassium plus either ammonium (NH_4^+) or hydronium (H_3O^+) ions, or water molecules in two different proportions. These atomistic models are optimized from first principles using plane waves and pseudo-potentials within the formalism of density functional theory (DFT). The resulting lattice lengths, lattice dynamics in the form of infrared frequencies, positions of interlayer molecules and simulated X-ray powder diffraction (XRPD) patterns are analyzed with reference to the available experimental data. We conclude that all four illite models display properties that fall within the range of available experimental data, and that therefore these are state-of-the-art atomistic illites, ready for use in further studies. Furthermore, the analytical data from these models will enable the characterization of physical samples of illite with varying interlayer constituents.

Keywords: DFT, shale, ammonium ions, hydronium ions, $2M_1$-illite, interlayer-deficient mica