Equations of state and elasticity of brucite and portlandite at high temperatures and pressures from classical atomistic simulations

Tararushkin E V[1,@] and Kalinichev A G[1,2]

[1] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

[2] Institut Mines-Télécom Atlantique, 4 Rue Alfred Kastler, Nantes 44300, France

[@] etararushkin@hse.ru

Brucite, $Mg(OH)_2$, and portlandite, $Ca(OH)_2$, have a similar hexagonal layered crystal structure that is held together by hydrogen bonding between the hydroxyl groups of the opposing layers. The thermodynamic and elastic properties of such minerals at high temperatures and pressures are of great importance for fundamental geochemistry and geophysics. The ClayFF force field [1] has been originally developed for classical atomistic computer simulations of clays and their hydrated interfaces under ambient conditions. Here we are using its new recent modification, ClayFF–MOH [2], more accurately accounting for the bending of Mg–O–H and Ca–O–H angles in the crystal structures, in order to test the applicability of this model at high temperatures and pressures well beyond the range of the original ClayFF implementation. The P–T dependencies of brucite and portlandite crystallographic parameters, the compressibility of their crystal lattices, the coefficients of thermal expansion, and the vibrational spectra are calculated in a series of classical molecular dynamics simulations using the ClayFF–MOH model. The research was supported by the HSE University Basic Research Program and used the NRU HSE supercomputer.

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