Classical atomistic simulations of the 10 Å phase at high temperatures and pressures

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The 10 Å phase, $Mg_3Si_4O_{10}(OH)_2 \cdot nH_2O$, is an important member of the family of dense hydrous magnesian silicates (DHMS) minerals is of great interest for fundamental geochemistry and geophysics. The ideal model of the 10 Å phase has already been successfully investigated by classical atomistic simulations [1]. However, more recent experiments show that tetrahedral silicate layers of real the 10 Å phase may contain a certain amount of the hydrogarnet-type structural defects [2], which would affect its properties, especially at high temperature and pressure.

The ClayFF force field [3] has been originally developed for classical atomistic computer simulations of clays and other layered minerals. Here we are using the most recent modification of the force field [3], which can now more accurately account for the bending of Mg–O–H angles in the mineral layers and Si–O–H angles of the hydrogarnet-type defects, to test the applicability and predictive capacity of this force field model at high temperatures and high pressures well beyond the range of its original implementation.

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