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Nanoconfined water in the 10-Å phase at subduction zone conditions: Classical and *ab initio* MD simulations up to 7 GPa and 800 K

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The so-called 10-Å phase is one of the dense hydrous magnesium silicates (DHMSs) playing an important role in many processes responsible for the water budget in the Earth's upper mantle near subduction zones. Its nominal composition is usually written as $Mg_3Si_4O_{10}(OH)_2 \times xH_2O$, and its structure is often described as that of talc with some amount of water present in the interlayer space (e.g., [1]). However, more recent experiments suggest that the silicate layers of the real 10-Å phase contain about 10% of hydrogarnet-type structural defects [2-4], which would affect its properties, especially at high temperatures and pressures. The silanol groups of the defects are forming hydrogen bonds to the interlayer H_2O molecules making the normally hydrophobic talc surfaces more hydrophilic.

Here we are using the most recent modification of the ClayFF force field [5], that can 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. The pressure and temperature dependencies of the 10-Å phase properties are calculated in a series of classical MD simulations and compared with *ab initio* results and a diverse set of available experimental data.

References

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