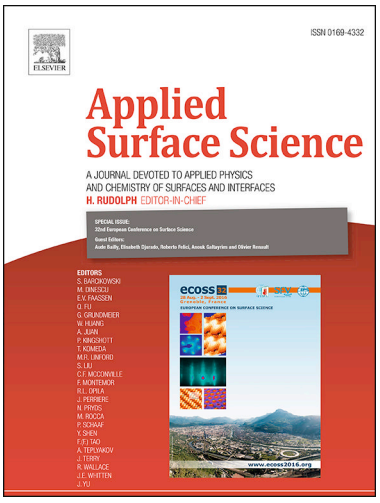

The surface stability and morphology of tobermorite 11 Å from first principles

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The surface stability and morphology of tobermorite 11 Å from first principles

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Abstract

Tobermorite minerals are important in many industrial processes typically occurring in hydrous environment. Their functionality is therefore governed in various aspects by their morphology and surface stability/reactivity. Here, we present the results of the surface energies and morphology of normal tobermorite 11 Å in a water vapor environment investigated by employing first principles atomistic thermodynamic calculations. For the low index tobermorite surfaces studied, the calculated surface energies fall within a narrow range (0.41–0.97 J/m^2) with the (004) surface being the most stable. The equilibrium morphology is a thin pseudohexagonal plate elongated along the b axis. The hydrated surfaces are more stable at high water vapor chemical potentials with the stability enhanced as the water partial pressures are varied from ambient to supercritical hydrothermal conditions. Increasing the water vapor chemical potential gives rise to a smaller size of the tobermorite crystal, with the equilibrium morphology remaining unaltered.

Keywords: Tobermorite, Ab initio, Surface Energy, Morphology, Chemical Potential

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