Density Functional Theory Calculations and Thermodynamic Analysis of the Forsterite Mg2SiO4(010) Surface

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The stability of possible termination structures for the (010) surface of forsterite, Mg2SiO4, is studied using a density functional theory (DFT)-based thermodynamic approach. The DFT calculations are used to estimate the surface Gibbs free energy of various surface structures and compare their stability as a function of the chemical environment. Among nine possible terminations, the SiO-II, M2, and O-II terminations are found to be most stable as conditions range from Mg-poor to Mg-rich. This relative stability order remains the same at elevated temperatures. The surface phase diagram obtained provides ground for further theoretical studies of chemical processes on forsterite surfaces in terrestrial planets.

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