Low-pressure analogs of $MgSiO_3$ post-perovskite at ultrahigh pressures by first principles

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$MgSiO_3$ post-perovskite (Mg-PPV) is the final form of this silicate in the Earth’s mantle. However, the fate of Mg-PPV in the mantle of terrestrial exoplanets, where pressures and temperatures are much higher than those on Earth, is still an open question. Knowledge of such transitions will be fundamental for numerical simulations of mantles in terrestrial exoplanets. Previously, by first principles, we predicted a complex series of phase transitions involving dissociation ($MgSiO_3$ -> Mg_2SiO_4 + $MgSi_2O_5$ -> Mg_2SiO_4 + SiO_2 -> MgO + SiO_2) and recombination (MgO + $MgSiO_3$ -> Mg_2SiO_4 or SiO_2 + $MgSiO_3$ -> $MgSi_2O_5$) reactions among silicates and elementary oxides. These transitions also depend on the chemical compositions of planetary mantles [1,2] and occur at very high pressure (above ˜0.5 TPa), which makes experimental validation rather difficult. Here, we search for these low-pressure analogs using first principles calculations. We hope the present study will facilitate experimental validation and encourage researchers of numerical simulations of mantles in terrestrial exoplanets to take dissociations and recombinations of Mg-PPV into account.

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