Effect of impurity on post-post-perovskite transition of $MgSiO_3$ by first principles

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Several computational studies have predicted post-post-perovskite transitions in MgSiO3 at ultrahigh pressures and temperatures which can occur at deep interiors of super-Earths: $MgSiO_3$ --> 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 + $MgSiO_3$ --> $MgSi_2O_5$) [1-5]. As demonstrated in a very recent numerical simulation, these transitions are crucially important in modeling interiors of super-Earths up to 20 times Earth’ s mass [6]. However, in the previous studies, these post-post-perovskite transitions were considered only for pure Mg-Si-O. In actual super-Earths, impurities, Fe, Al, or so forth, should exist. Here we will investigate effects of impurities on post-post-perovskite transitions: transition pressures, local atomic structures, and equation of states.

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