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 MgSiO$_3$ at ultrahigh pressures and temperatures which can occur at deep interiors of super-Earths: MgSiO$_3$ $\rightarrow$ Mg$_2$SiO$_4$ + MgSi$_2$O$_5$ $\rightarrow$ Mg$_2$SiO$_4$ + SiO$_2$ $\rightarrow$ MgO + SiO$_2$) and recombination (MgO + MgSiO$_3$ $\rightarrow$ Mg$_2$SiO$_4$ or SiO$_2$ + MgSiO$_3$ $\rightarrow$ MgSi$_2$O$_5$) [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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