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Post-perovskite phase boundary of Fe- and Al-bearing MgSiO3
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The post-perovskite (PPv) phase transition of $MgSiO_3$ bridgmanite (Br) [1,2,3] occurs in the pressure (P) and temperature (T) conditions corresponding to the Earth's D? layer. Therefore, $MgSiO_3$ PPv is believed to be a key mineral to understanding the seismological properties in this layer. However, to date, it is still a challenging subject to determine the phase transition boundary preciously in the geophysically relevant Fe and Al-bearing compositions. Based on the first-principles methods combined with the internally consistent LSDA+*U* method and the lattice dynamics approach, the high-P and high-T thermodynamics of the $MgSiO_3$ phases are directly calculated with incorporation of 6.25 mol% of Fe^{2+}, $Fe^{3+}Fe^{3+}$, $Fe^{3+}Al^{3+}$, and $Al^{3+}Al^{3+}$ [4,5]. Using calculated free energies, we determine the PPv phase boundaries for Fe and Al-bearing compositions. Our results show that at 2500 K, the $Fe^{3+}Al^{3+}$ and $Fe^{3+}Fe^{3+}$ incorporations span coexisting domains between Br and PPv significantly with lowering the transition pressure, in contrast to the Fe^{2+}- and $Al^{3+}Al^{3+}$-bearing cases.

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