Effects of Fe and Al incorporations on MgSiO$_3$ postperovskite phase boundary

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MgSiO$_3$ bridgmanite (Br) will undergo a post-perovskite (PPv) phase transition$^{[1,2,3]}$ in the pressure ($P$) and temperature ($T$) conditions corresponding to the Earth’s D” layer. Therefore, the phase change is recognized as the key for understanding the seismological observations in the D” layer. However, to date, it is still a challenging subject to determine the phase transition boundary precisely 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-$P,T$ 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$^{3+}$, and 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, incorporations of Fe$^{3+}$, Fe$^{3+}$, and Fe$^{3+}$, Al$^{3+}$ span coexisting domains between Br and PPv significantly with lowering the transition pressure, in contrast to the Fe$^{2+}$ and Al$^{3+}$-bearing cases.

References:

Keywords: First-principles method, internally consistent LSDA+$U$, MgSiO$_3$, postperovskite