Thermodynamic properties of Mg-postperovskite with Fe$^{3+}$ and Al$^{3+}$ dopant: an internally consistent LSDA+U study

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Thermodynamic properties of MgSiO$_3$ perovskite (Pv) and postperovskite (PPv) with Fe and Al incorporation at high pressure and high temperature are important to understand the Earth’s lower mantle (LM). The thermodynamic properties of Fe$^{2+}$, Fe$^{3+}$, and Al$^{3+}$-bearing Pv[1,2,3] and Fe$^{2+}$-bearing PPv[4] have been investigated in our previous works uniformly based on first-principles method combined with the internally consistent LSDA+$U$ method and quasi-harmonic approximation (QHA). However, to date, effects of trivalent ions, Fe$^{3+}$ and Al$^{3+}$, on the thermodynamic properties of PPv are still unclear. In this work, by using the same methods with previous works, the structural, electronic, magnetic, and thermodynamic properties of (Mg,Fe$^{3+}$)(Si,Fe$^{3+}$)O$_3$ and (Mg,Fe$^{3+}$)(Si,Al$^{3+}$)O$_3$ PPv at several pressures, from 0 GPa to 180 GPa, are investigated. Our results show that for (Mg,Fe$^{3+}$)(Si,Fe$^{3+}$)O$_3$ PPv, Fe$^{3+}$ ions substituted at Mg and Si site respectively have the high and low spin state within the deep LM pressure range, while Fe$^{3+}$ in (Mg,Fe$^{3+}$)(Si,Al$^{3+}$)O$_3$ PPv remains in the high spin state. Furthermore, separated phase between Fe$_2$O$_3$ and Al$_2$O$_3$ in PPv is found unfavorable.

References:

Keywords: First-principles method, Internally consistent LSDA+$U$, Thermodynamic properties, Postperovskite