

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 $(\text{Mg},\text{Fe}^{3+})(\text{Si},\text{Fe}^{3+})\text{O}_3$ and $(\text{Mg},\text{Fe}^{3+})(\text{Si},\text{Al}^{3+})\text{O}_3$ PPv at several pressures, from 0 GPa to 180 GPa, are investigated. Our results show that for $(\text{Mg},\text{Fe}^{3+})(\text{Si},\text{Fe}^{3+})\text{O}_3$ 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 $(\text{Mg},\text{Fe}^{3+})(\text{Si},\text{Al}^{3+})\text{O}_3$ PPv remains in the high spin state. Furthermore, separated phase between Fe_2O_3 and Al_2O_3 in PPv is found unfavorable.

References:

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