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

Xianlong WANG\(^1\), Taku TSUCHIYA\(^1\) (1.GRC, Ehime University and ELSI, Tokyo Institute of Technology)

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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: