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Investigation on thermodynamic properties of Fe- and Al-bearing MgSiO3 perovskite: an internally consistent LSDA+U study
Investigation on thermodynamic properties of Fe- and Al-bearing MgSiO3 perovskite: an internally consistent LSDA+U study

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Researchers have extensively focused on behaviors of iron (Fe) in Fe-bearing $MgSiO_3$ perovskite (Pv) and postperovskite (PPv) at high pressure and high temperature to better understand the thermodynamic properties of the Earth's lower mantle (LM). Effects of Fe^{2+} and Fe^{3+} on the thermodynamic properties of Pv and PPv were already clarified in our previous work through first-principles simulations [1,2,3]. However, corresponding effects of aluminum (Al), which is believed to be another important impurity in the LM minerals and can increase the concentration of Fe^{3+} significantly in silicate Pv, are still not clear. In this work, by taking use of first-principles method combined with the internally consistent LSDA+*U* method and quasi-harmonic approximation (QHA), the thermodynamic properties of Fe- and Al-bearing Pv under several pressures, from 0 GPa to 180 GPa, are investigated. At the beginning, we will discuss stability of the structures and spin-configurations of Fe^{3+} and Al^{3+}-bearing Pv. Our results show that the configuration with high-spin Fe^{3+} substituted at the Mg site, while Al^{3+} located at its neighboring Si site, has the lowest enthalpy through the whole LM pressure range, showing that the spin transition of Fe^{3+} co-doped with Al^{3+} in Pv is highly unlikely under LM conditions. Then, based on the structural stability, the thermodynamic properties of Fe^{3+}- and Al^{3+}-bearing Mg Pv will be discussed.

キーワード: First-principles method, internally consistent LSDA+U, thermodynamic properties, Fe- and Al-bearing Mg Pv
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