

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

Xianlong Wang^{1*}, Taku Tsuchiya¹

¹Geodynamics Research Center, Ehime University

Researchers have extensively focused on behaviors of iron (Fe) in Fe-bearing MgSiO₃ 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 Fe²⁺ and Fe³⁺ 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 Fe³⁺ 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 Fe³⁺ and Al³⁺-bearing Pv. Our results show that the configuration with high-spin Fe³⁺ substituted at the Mg site, while Al³⁺ located at its neighboring Si site, has the lowest enthalpy through the whole LM pressure range, showing that the spin transition of Fe³⁺ co-doped with Al³⁺ in Pv is highly unlikely under LM conditions. Then, based on the structural stability, the thermodynamic properties of Fe³⁺- and Al³⁺-bearing Mg Pv will be discussed.

Keywords: First-principles method, internally consistent LSDA+U, thermodynamic properties, Fe- and Al-bearing Mg Pv