Oral | Symbol S (Solid Earth Sciences) | S-MP Mineralogy & Petrology

[S-MP47_1PM1]Physics and Chemistry of Minerals

Convener:*Hiroki Okudera(School of Natural System, College of Science and Engineering), Atsushi Kyono(Graduate School of Life and Environmental Sciences, University of Tsukuba), Chair:Hiroki Okudera(School of Natural System, College of Science and Engineering), Hiroshi Kojitani(Department of Chemistry, Faculty of Science, Gakushuin University)

Thu. May 1, 2014 2:15 PM - 4:00 PM 422 (4F)

In this session, we discuss about Earth and planetary materials (including amorphous and melts) with the results obtained from various experimental methods such as X-ray, FT-IR, Raman, computer simulation and so on.

3:45 PM - 4:00 PM

[SMP47-P01_PG]Thermodynamic properties of Mg-postperovskite with Fe^{3+} and Al^{3+} dopant: an internally consistent LSDA+U study

3-min talk in an oral session

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

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 uniformally 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_2O_3 and Al_2O_3 in PPv is found unfavorable.References:[1] Metsue, A. and Tsuchiya, T. (2012) Geophys. J. Int. **190**, 310.[2] Tsuchiya, T. and Wang, X. (2013) J. Geophys. **118**, 83.[3] Wang, X. and Tsuchiya, T. To be submitted.[4] Metsue, A. and Tsuchiya, T. (2011) J. Geophys. Res. **116**, B08207.