

# The 406th Geodynamics Seminar

## Post-perovskite phase boundary of Fe- and Al-bearing MgSiO<sub>3</sub>

Dr. Xianglong Wang (JSPS Postdoctoral Fellow, GRC)

Date: 01.23.2015 (Fri) 16:30 ~

Venu: Meeting Room #486, Science  
Research Bldg 1, Ehime Univ.

日時: 2015年1月23日(金) 16:30~

場所: 愛媛大学 総合研究棟 I  
4階 共通会議室



### Abstract

The post-perovskite (PPv) phase transition of MgSiO<sub>3</sub> bridgmanite (Br) occurs in the pressure (P) and temperature (T) conditions corresponding to the Earth's D'' layer. Therefore, MgSiO<sub>3</sub> PPv is believed to be a key mineral to understanding the seismological properties in this layer. However, to date, it is still a challenging subject to determine the phase transition boundary precisely in the geophysically relevant Fe and Al-bearing compositions. Based on the first-principles methods combined with the internally consistent LSDA+*U* method and the lattice dynamics approach, the high-P and high-T thermodynamics of MgSiO<sub>3</sub> are directly calculated with incorporation of 6.25 mol% of Fe<sup>2+</sup>, Fe<sup>3+</sup>Fe<sup>3+</sup>, Fe<sup>3+</sup>Al<sup>3+</sup>, and Al<sup>3+</sup>Al<sup>3+</sup>. Using calculated free energies, we determine the PPv phase boundaries for Fe and Al-bearing compositions. Our results show that at 2000 K, the Fe<sup>3+</sup>Al<sup>3+</sup> and Fe<sup>3+</sup>Fe<sup>3+</sup> incorporations span coexisting domains between Br and PPv significantly with lowering the transition pressure, in contrast to the Fe<sup>2+</sup>- and Al<sup>3+</sup>Al<sup>3+</sup>-bearing cases.