INTERNATIONAL FRONTIER SEMINAR № 082

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Venue: Zoom

A link will be sent @grc-all within 30 minutes before the beginning of the seminar.

Temperature-induced order-disorder phase transition in the Mg-Si-O post-post-perovskite system by first principles

The highest-pressure form in the Earth of the major mantle silicate $MgSiO_3$-bridgmanite is post-perovskite (PPV). Knowledge of the fate of PPV at higher pressures relevant for super-Earth-type planets is fundamental for us to start modeling the internal structure and dynamics of these planets. First principles studies so far predicted that $MgSiO_3$ PPV undergoes the pressure-induced three-stage dissociations: $MgSiO_3$ PPv → Mg_2SiO_4 + $MgSi_2O_5$ → Mg_2SiO_4 + SiO_2 → MgO + SiO_2 up to 4 TPa [1-3]. In these post-PPV Mg_2SiO_4 and $MgSi_2O_5$, oxygen arrangements around Mg and Si are very similar, expecting us new phase transitions which should be induced by temperature due to configurational entropy. Very recently, indeed, we predicted another type of phase transition, i.e., a temperature-induced order-disorder transition (ODT) in I-42d-type Mg_2GeO_4, a low-pressure analog of Mg_2SiO_4 [4]. In this talk, we will newly predict the similar ODT transitions in Mg_2SiO_4 and $MgSi_2O_5$ by first principles Boltzmann ensemble statistics calculations. We will calculate full phase boundaries of the post-PPV transitions in Mg-Si-O within the QHA. The predictions here will be quite important for modeling mantle dynamics in large super-Earths.

[1] S. Q. Wu et al., J. Phys.: Condens. Matter, 26, 035402 (2014).
[2] H. Niu et al., Scientic Reports 5, 18347 (2015).
[3] K. Umemoto et al., Earth Planet. Sci. Lett. 478, 40-45 (2017).
[4] K. Umemoto and R. M. Wentzcovitch, Phys. Rev. Materials 5, 093604 (2021).

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