THE GEODYNAMICS SEMINAR Nº 569

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## Venue: Zoom

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

# An ab initio approach to the lattice dynamics of cubic $CaSiO_3$ perovskite

$CaSiO_3$ perovskite (CaPv) is expected to be the third most abundant phase in the Earth's lower mantle and a major one in the subducted basaltic crust. A cubic form of CaPv is believed to be stable under lower mantle temperature (T) and pressure (P) conditions. While its equilibrium properties such as thermoelasticity have been extensively studied, research on the thermal conductivity (κ), a non-equilibrium physical quantity, is almost absent due to technical difficulties both in theory and experiment. The κ of cubic CaPv may play a certain role as a source for controlling the temperature structure in the subducted basaltic crust and the heat transport property at the lowermost mantle, but to date the details are still unclear. Although the phonon frequencies dynamically stable is required to proceed with the computation of κ, a widely used ab initio technique, density-functional perturbation theory (DFPT), can fail to capture the high-T phase's thermodynamic stability, which leads to difficulty in the determination of the κ. To tackle this problem, I have recently initiated an ab initio molecular dynamics simulation based on the T-dependent effective potential method (Hellman+2011). This approach can take into account the T-effect on the force field unlike the DFPT scheme and could be a promising way to describe the stabilization of the soft-modes under high-T. In this presentation, I will show the preliminary results on the phonon property under lower mantle P and T conditions and discuss the method's applicability as a first step toward computing the κ.

**Keywords:** 1. Lower mantle
2. $CaSiO_3$
3. Lattice dynamics