



INSTITUT DE MINERALOGIE, DE PHYSIQUE DES MATERIAUX ET DE COSMOCHIMIE

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SÉMINAIRE

Jeudi 10 Juillet, 14 h

*Salle de Conférence, 4^e étage, Tour 22-23, Salle 1
IMPMC, Université P. et M. Curie, 4, Place Jussieu, 75005 Paris*

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AB INITIO MODELING OF THE COMPOSITIONAL AND THERMAL PROPERTIES OF THE EARTH'S LOWER MANTLE

Recent progress in theoretical mineral physics based on the density functional quantum mechanical computation method has been dramatic. It is now possible to predict finite-temperature equation of state and phase stability of complex minerals quantitatively with uncertainties that are comparable to or sometimes even smaller than those attached in experimental data under extreme condition.

Combining several techniques, we are trying to clarify compositional and thermal properties of the Earth's lower mantle. Some known lithology or mineralogy are examined through reproducibility test of seismological observations using finite-temperature elasticity data, which are obtained based on *ab initio* lattice dynamics method and internally-consistent LDA+U method for iron-bearing phases. Thermal property is then modelled for the likely lithology using lattice thermal conductivity data, which are obtained based on anharmonic lattice dynamics method.