

Harvard University -- Solid Earth Physics Seminar

Wednesday 12 December 2012, 12:00 pm

4th Floor Faculty Lounge, Hoffman Laboratory, 20 Oxford St.

Ab Initio Lower Mantle Model

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Recent progress in theoretical mineral physics based on the ab initio quantum mechanical computation method has been dramatic in conjunction with the rapid advancement of computer technologies. It is now possible to predict stability and several physical properties of complex minerals quantitatively with uncertainties that are comparable to or even smaller than those attached in experimental data. Our present challenges include calculations of transport properties such as lattice thermal conductivity. In this seminar, I will show a latest ab initio model of the Earth's lower mantle (LM) constructed based on our recent achievements. Topics will cover (1) mineralogy of the current LM with some insights into the subducted crustal materials, obtained by interpreting seismological observations, and (2) a further extension to the thermal property, in particular, in the core-mantle boundary region, which has great influences on the evolution of the deep Earth.