Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Computation of the Iron and Iron-Nickel Phase Diagrams from Ambient to Earth's Inner Core XUAN LUO, R.E. COHEN, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015 — We have performed first-principles computation for the magnetic iron and iron-nickel over a wide range of pressure (0-400GPa) and temperature (0-6000K), within density-functional theory (DFT) in the generalized-gradient approximation using the projector augmented wave (PAW) method with the ABINIT code. We computed the free energies of hcp, bcc and fcc phases for iron and nickel including the thermal excitation of electrons and quasiharmonic phonons computed using the supercell method. We find that at high temperatures and pressures random stacking of fcc and hcp (rhcp) is most stable since the difference in Gibbs free energy between fcc and hcp Fe is smaller than the thermal energy. We computed the free energy of stacking faults, the rhcp phase and the percentage of fcc and partial ordered sequences along the melting curve. For the first time, we used first-principles calculation to be able to produce the pure-Fe phase diagram including the magnetic contributions at low pressures. In the Fe-Ni system, we find that FeNi3 is an intermediate phase below 700K at 0 GPa, consistent with experiment, and below 50 GPa at 0K. Finally, we obtained the T-P-x phase diagram for FeNi from 0-400 GPa and 0-6000K.

Xuan Luo
Geophysical Laboratory, Carnegie Institution of Washington,
Washington, DC 20015

Date submitted: 17 Dec 2008 Electronic form version 1.4