Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Pressure Correction of Density Functional Theory Calculations

SHUN HANG LEE, JONES TSZ-KAI WAN, The Chinese University of Hong Kong

— The modern implementation of density functional theory algorithms involves approximations in the exchange correlation, which leads to discrepancies between experimental measurements and theoretical predictions. In this talk, we present a comparison of exchange correlation approximations by performing first-principles calculations on bulk structures such as MgO, MgSiO3 perovskite and post-perovskite at pressures up to deep Earth conditions. For a given structure, the calculated results such as the equation of state and bulk modulus corresponding to each exchange correlation are compared. At each volume, the pressure estimated by generalized gradient approximation (GGA) is usually above that by local density approximation (LDA,) resulting in a shift in the equations of states. At ambient conditions, such pressure difference is almost independent of pressure and temperature. However, at extreme pressure and temperature such as planetary interiors, this difference becomes temperature and pressure dependent and could lead to large errors in the predictions of properties for minerals at such conditions. In our study, we quantified such a pressure difference at different volume and temperature.

Shun Hang Lee
The Chinese University of Hong Kong

Date submitted: 02 Dec 2007 Electronic form version 1.4