Structure phases of MgSiO$_3$ in Earth’s lower Mantle: ab initio calculations

MOHAMMED SAHNOUN, PATRIC OULEVEY, Department of Chemistry, University of Fribourg, CH-1700 Fribourg, Switzerland, BERNARD GROBÉTY, Department of Mineralogy, University of Fribourg, CH-1700 Fribourg, Switzerland, CLAUDE DAUL, Department of Chemistry, University of Fribourg, CH-1700 Fribourg, Switzerland — The Earth’s mantle is divided into five layers with four major phase transitions at 410, 520, 660 and ∼2600-km depths, due to a structural and chemical changes of its main constituent minerals. MgSiO$_3$ is believed to be a predominant mineral, at least in the upper part of the lower mantle. MgSiO$_3$ has a structural sequence from corundum-type ilmenite to CaIrO$_3$-type structure ($Cmcm$ symmetry). First-principles calculations have been performed within the full-potential linearised augmented plane-wave method (FP-LAPW). We calculated equilibrium lattice parameters at different pressures up to 150 GPa. Four crystal structures relevant to MgSiO$_3$ were considered and they can grouped in two pairs of distinct types: (a) corundum-like and Rh$_3$O$_3$(II) structure-like, and (b) perovskite and CaIrO$_3$ structure-like. To investigate the structural phase transitions in MgSiO$_3$, we calculated the enthalpy (E+PV) of the four-structures as a function of pressure from 0 to 150 GPa. The intersection of the curves indicates which structure is more stable and gives the transition pressure.

Mohammed Sahnoun
Department of Chemistry, University of Fribourg, CH-1700 Fribourg, Switzerland

Date submitted: 15 Jan 2006
Electronic form version 1.4