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**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 $Rh_2O_3$(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.

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