

## **High-pressure phase transitions in MgSiO<sub>3</sub> orthoenstatite studied by atomistic computer simulation**

**SANDRO JAHN\***

GeoForschungsZentrum Potsdam, Department 4, Telegrafenberg, 14473 Potsdam, Germany

### **ABSTRACT**

Molecular dynamics simulations and first-principles electronic structure calculations are used to study the structural behavior of orthoenstatite, MgSiO<sub>3</sub>, at high pressures. The calculations suggest two possible high-pressure polymorphs of orthoenstatite, one with *P2<sub>1</sub>ca* and the other with *Pbca* symmetry. Both polymorphs are structurally related to orthoenstatite. Molecular dynamics simulations reveal the displacive nature of the phase transitions between the three phases. Electronic structure calculations predict a phase transition from orthoenstatite to the metastable *P2<sub>1</sub>ca* structure at 9 GPa, which may explain the anomalies in elastic and vibrational properties observed experimentally. A second metastable transition from the *P2<sub>1</sub>ca* to the high-pressure *Pbca* structure may be observable above 20 GPa.

**Keywords:** DFT, MD simulation, enstatite, phase transition, high pressure