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High-pressure phase transitions in $MgSiO_3$ orthoenstatite studied by atomistic computer simulation

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ABSTRACT

Molecular dynamics simulations and first-principles electronic structure calculations are used to study the structural behavior of orthoenstatite, $MgSiO_3$, at high pressures. The calculations suggest two possible high-pressure polymorphs of orthoenstatite, one with $P2_1ca$ 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 $P2_1ca$ structure at 9 GPa, which may explain the anomalies in elastic and vibrational properties observed experimentally. A second metastable transition from the $P2_1ca$ to the high-pressure *Pbca* structure may be observable above 20 GPa.

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