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Ab initio study of $MgSiO_3$ low-clinoenstatite at high pressure

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ABSTRACT

We investigated the athermal high-pressure behavior of the structural properties of $MgSiO_3$ low clinoenstatite using the plane wave pseudopotential method within the local density approximation. The experimental zero pressure structure and pressure variations of the lattice parameters were reasonably well reproduced. The calculated atomic positions vary slightly and monotonically with pressure. Our results showed that MgO_6 octahedra are three times more compressible than SiO_4 tetrahedra, consistent with the general observation that the SiO_4 tetrahedra are nearly incompressible in silicates. $Mg2O_6$ octahedra (the larger of two Mg sites) remain most distorted over the pressure regime studied while $Mg1O_6$ octahedra and both types of SiO_4 tetrahedra show similar level of distortions. The tetrahedral chain angles were shown to slightly vary with pressure indicating that the structure under compression always remains highly distorted away from the ideal close-packing of O atoms.