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First principles calculations on the high-pressure behavior of magnesite

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ABSTRACT

The equation of state and high pressure (>200 GPa) behavior of magnesite were investigated using first principles pseudopotential calculations based upon density functional theory within the generalized gradient approximation. Using a third-order Birch-Murnahan equation, the calculations predict a bulk modulus $K_T(0) = 99.0(5)$ GPa with a $\partial K/\partial P = 4.28(1)$; with a fixed $\partial K/\partial P = 4$, the $K_T(0)$ is 111(1) GPa. The results show very good agreement with recent experimental data. The simulations also confirm experimental studies which show that the CO_3 groups are rigid incompressible units while the Mg-O bond length undergoes significant compression. The fully relaxed calculations show no phase transition within this pressure range, and therefore magnesite may be stable throughout the lower mantle subject to temperature destabilization.