Thermodynamic and structural properties of dolomite under high pressures and temperatures from ab initio calculations

Rykounov A A

Federal State Unitary Enterprise "Russian Federal Nuclear Center—Academician Zababakhin All-Russian Research Institute of Technical Physics", Vasilieva 13, Snezhinsk, Chelyabinsk Region 456770, Russia

arykounov@gmail.com

Pseudopotential-based *ab initio* approaches were used to calculate thermodynamic and structural properties of calcium–magnesium carbonate $CaMg(CO_3)_2$ found as dolomite in the nature. Calculations were done for densities from 1.0 to 8.0 g/cm^3 and temperatures from 0 to 60 kK. The dependence of calculated results on the particular form of the exchange-correlation functional and parameters of the quantum molecular dynamics method was investigated. Isotherms were constructed for different polymorphic modifications of dolomite and their relative stability was evaluated. Calculated data on static and dynamic compressibility were compared with experimental data.