Thermodynamic Properties of $CaSiO_3$ Perovskite at High Pressure and High Temperature

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The thermodynamic properties of tetragonal $CaSiO_3$ perovskite are predicted at high pressures and temperatures using the Debye model for the first time. This model combines the ab initio calculations within local density approximation using pseudopotentials and a plane wave basis in the framework of density functional theory, and it takes into account the phononic effects within the quasi-harmonic approximation. It is found that the calculated equation of state is in excellent agreement with the observed values at ambient condition. Based on the first-principles study and the Debye model, the thermal properties including the Debye temperature, the heat capacity, the thermal expansion and the entropy are obtained in the whole pressure range from 0 to 150 GPa and temperature range from 0 to 2000 K.

Key words: Thermodynamic Property; High Pressure; First Principles.
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