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Effect of temperature on the thermodynamic properties of $Na_2Ti_3O_7$ HONG ZHANG, College of Physical Science and Technology, Sichuan University, China, HAIYING WU, Atomic and Molecular Institute, Sichuan University, China, ATOMIC AND MOLECULAR COMPUTATIONAL GROUP TEAM
— The equilibrium structure of the compound $Na_2Ti_3O_7$ has been obtained via the minimization of the total energy within Local Density Approximation (LDA) based on Density Functional Theory (DFT), the calculated equilibrium volume are in agreement with available experimental values. In the meantime, the thermodynamic properties are investigated applying nonempirical Debye-like model combining with the first principle theory in the quasi-harmonic approximation. The evaluated equilibrium volume using this model agrees with the values from *ab intio* and from experiment. Our results demonstrate that this method can provide reliable predictions for the temperature dependence of these quantities such as the equation of state, the bulk modulus, the heat capacity, and the thermal expansion in detail. And our calculated thermodynamic properties are all in agreement with available experimental data.

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