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The behavior of system temperature, volume, enthalpy, and total energy of ZnO wurtzite phase under different temperature and pressure, a molecular dynamics prediction

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The dl_poly_4 software and Parallel Molecular Dynamics are investigated to analyze the behavior of system temperature, volume, enthalpy, and total energy of ZnO wurtzite phase under an extended temperature and pressure. In this work we study the effect of the temperature and pressure in the range of 300-3000K and 0-200GPa respectively on the system temperature, volume, enthalpy, and total energy.The interatomic interaction is modeled by the Coulomb-Buchingham pair potential, where we confirmed its validity. Our data are in agreement with some available results due to no more work under the previous extreme conditions of pressure and tempearture. Tis work has great importance in pharmacy, medecine, nanotechnology industry and in geophysics, but needs confirmation in future.

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