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Evolution in time of total energy and molar volume of ZnO wurtzite phase under different temperatures and pressures, a molecular dynamics prediction

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The relationship between isothermal, isobaric ensemble, total energy, molar volume and its evolution in time under low and high temperature and pressure have been investigating using molecular dynamics and the DL Poly 4 software (RAVEN supercomputer, Wales Cardiff University). In this work we used an extended temperature and pressure in the range of 300-3000K and 0-200GPa respectively for ZnO wurtzite phase in order to analyse the behaviour of evolution in time of total energy and molar volume. Our data confirm the validity of the interatomic potential under ambient conditions, which is closed to some available work, due to no more studies under previous ranges. We found a homogeneous of our results of extended conditions of temperature and pressures, with the ambient conditions that confirm the validity of the potential and therefore the agreement of our work. This data permit to know the behaviour of ZnO wurtzite phase and in other work the phase transitions values in each isobaric and isothermal ensemble, also these results have great importance in technology and nanotechnology especially in the field of medicine, pharmaceuticals and geophysics. However, these results are only a simulation prediction which needs an experimental confirmation in future.

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