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The enthalpy behavior of ZnO wurtzite phase under isothermal and isobaric ensemble a molecular dynamics prediction

In this work, we investigated parallel molecular dynamics technique and DL_POLY software to study ZnO wurtzite phase in an isothermal and isobaric ensemble under different temperature and pressure, 300-300 K and 0-200 Gpa respectively. The calculations were done in the supercomputer of Cardiff University in UK. In this work, we analysed the behavior of enthalpy of system; evolution in time of simulation 300 ps, the effect of pressure and temperature on the enthalpy and the equilibrium time versus pressure. Our results are in agreement with some available date, due to no more results for comparison under the previous extreme conditions of pressure and temperature. Our results have a great importance especially in medicine, pharmacy and in geophysics also in nanotechnology.

Biography

Yahia Chergui is a permanent Teacher in Institute of Electrical & Electronic Engineering. His research field is Condensed Matter using Molecular Dynamics and DI_Poly software.

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