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 behavior of evolution in time of total energy and molar volume. Our data comfirm 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 an 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 behavior 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, pharmaceutics and geophysics.

However these results are only a simulation predictions which needs an experimental confirmation in future.

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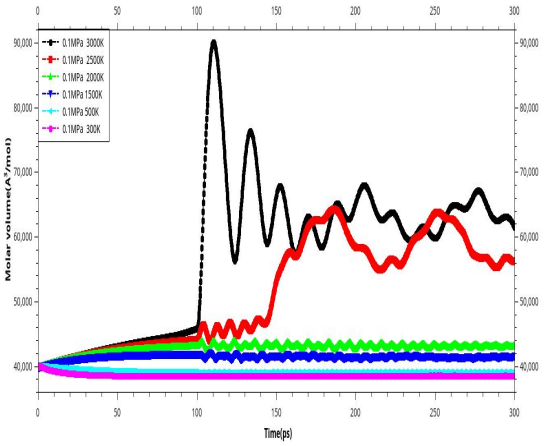


Figure1: Molar volume versus time under low pressure and different temperature

Biography



Yahia CHERGUI has completed his PhD from Badji Mokhtar University in Annaba, Algeria, he did his work of PhD in Cardiff University in UK.. His research field is Physics(condensed matter, simulation by molecular dynamics). He is a lecturer in Boumerdes University(Electrical & Electronics Engineering Institute) since 2012. He has published more than 7 papers in reputed journals and has been serving as a referee with condensed matter journal (IOP), Energy journal (Elsevier), and recently accepted to be a reviewer of *American Journal of Modern Physics.* He did all his PhD work in Cardiff University in UK.

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