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Abstract

Wurtzite Phase Transition of Zinc Oxide Using Equilibrium time of Total Energy and Volume a Molecular Dynamics Prediction.

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Abstract:

In order to confirm the phase transition of ZnO wurtzite phase, we use the equilibrium time of total energy and volume as a new method. We investigated molecular dynamics technique and dlpoly_4 to for our calculations. Our system is 2916 atoms of Zn+2 and O-2 in a simulation box of 9x9x9, where this system is used in isothermal and isobaric ensemble in the range of 300-3000K and 0-200GPa. The calculation ran in the supercomputer RAVEN of Cardiff University. Although no more study at these conditions of pressure and temperature, our work is in agreement with available data, the rest need an experimental confirmation in future. These results have a huge importance in pharmacy, medicine, nanotechnology and geophysics.

Biography:

Yahia CHERGUI has completed his PhD from Badji Mokhtar University in Annaba, Algeria. 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 9 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. He is an academic member of the Athens Institute for Education and Research belonging to Physics Unit.

Recent Publications:

1. Yahia Chergui, et al Mater. Res. Express, 2017.
2. Yahia Chergui, et al Journal of Material Sciences, 2013.
3. Yahia Chergui, et al MSAIJ, 2012.
4. Yahia Chergui, et al Journal of Electron Devices, 2011.
5. Yahia Chergui, et al Eur. Phys. J. Appl. Phys, 2010.
6. Hovhannisyan AA, et al Bioorg Med Chem Lett, 2017

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