Evolution in Time of Total Energy of ZnO Rocksalt Type a Molecular Dynamics Computation

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Abstract

Total energy of ZnO rocksalt type is investigated using Molecular Dynamics technique and DL_POLY_4. The calculations of this work ran on RAVEN Supercomputer of Cardiff University in UK. In this work we analyze the evolution in time of total energy under different temperatures and pressures; the range of pressure is 0-100GPa and of temperature is 300-3000K. The interatomic interactions are modeled by Buckingham-Coulomb potential. The results of our work are in agreement with available theoretical and experimental data. This work has a great importance in Nanotechnology and different sectors of industry.

Biography:

Yahia CHERGUI has completed his PhD from Badji Mokhtar University in Annaba, Algeria. All the work of his PhD did in Cardiff University in UK during 6 months. 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 is an academic member of the Athens Institute for Education and Research belonging to Physics Unit.

References

1. Determination of organic solar cell parameters based on single or multiple pin structures
2. Vacuum 84 (2), 326-329 2009
3. Comparative study of dye-sensitized solar cell based on ZnO and TiO2 nanostructures
4. Solar Cells-Dye-Sensitized Devices 2011
5. A new model for extracting the physical parameters from IV curves of organic and inorganic solar cells
6. Solar Cells, 53 2011

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