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Abstract

Effect of Different Pressures and Temperatures on Electronics Band of ZnO a Molecular Dynamics Predictions.

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Abstract:

Parallel molecular dynamics becomes today a powerful tool to investigate physical properties prediction. In this work we use this technique of simulation and dl_poly_4 software in Raven supercomputer(Cardiff University, UK) to analyse the effect of pressures and temperatures on the electronics band between ZnO atoms, where we choose a system of 2916 atoms of Zn+2 and O-2 in a simulation box of 9x9x9. The range of pressure is between 0-200GPa and for temperature is 300-3000K, an isothermal and isobaric system are used of our simulation. Our work has an agreement with some available data due to no more information under previous conditions of pressure and temperature. This work has an important value on nanoscale properties in order to use it in macroscale properties.

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.

Recent Publications:

- Yahia Chergui, Chaos, 2019
- Yahia Chergui, Chem Cent J, 2018
- Yahia Chergui, Biol Res, 2017.
- Yahia Chergui, Nature, 2016
- Yahia Chergui, Appl Microbiol Biotechnol, 2015

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