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Abstract

Equilibrium Time of System Temperature and Phase Transition Under High and Low Pressure and Temperature of ZnO Wurtzite Structure, a Molecular Dynamics Prediction

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Abstract:
The parallel molecular dynamics and dlpoly_4 are investigated to study the equilibrium time of system temperature of ZnO wurtzite phase under low and high temperatures and pressures using the range of 300-3000K and 0-200GPa respectively. The interatomic interaction is modelled by Buckingham-Coulomb potential, we analysed the equilibrium time of system temperature and system temperature evolution under different pressures and temperatures. Our work is in agreement with available data, which confirm the phase transition from the wurtzite phase to rocksalt .We tried to confirm that the equilibrium time of system temperature versus pressure can give the transition pressure. This technique needs more work for confirmation. Our results are important in industry, medicine, pharmacy, nanotechnoly, and geophysics.

Biography:
Yahia CHERGUI is a lecturer in Electrical & Electronics Engineering Institute, Boumerdes Algeria. He has completed his PhD from Badji Mokhtar University in Annaba, Algeria. He did all his PhD work 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 many published articles and international conferences. He has been serving as a referee with condensed matter journal

Publication of speakers:

- Y. CHERGUI and D. E. MekkiTandem and single organic solar cells parameters evaluation from illumination I-Vplot
- Journal of Electron Devices, Vol. 11, 2011, pp. 515-520
- Y. CHERGUI and D. E. Mekki.Determination of organic solar cell parameters based on single ormultiple pin structures,Vacuum 84 (2010) 326-329.
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- Y. CHERGUI, N. Nehaoua and D. E. MekkiChapitre Solar Cells / Book 2 (first editin July 2011, InTec), ISBN979-953-307-191-5.Comparative study of dye-sensitized solar cell based on ZnO and TiO2: parametersevaluation,Edited by Prof. Leonid Kosyachenko Yuriy Fedkovych Chernivtsi NationalUniversity, Optoelectronics Department, Ukraine.
- Y. CHERGUI and D. E. MEKKIChapitre Solar Cells / Book 3 (first edition July2011, InTec), ISBN 9-953-307-192-2A New Model for Extracting the Physical Parameters from I-V Curves of Organic andInorganic Solar Cells Edited by Prof. Leonid Kosyachenko Yuriy Fedkovych Chernivtsi NationalUniversity
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