



# Effect of Temperature on Molar Volume of ZnO Wurtzite Phase Under Extended Pressure and Temperature a Molecular Dynamics Prediction

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## Abstract:

The behavior of molar volume of ZnO wurtzite phase is investigated using parallel molecular dynamics and dl\_poly\_4 software in RAVEN supercomputer of Cardiff University (UK). In this work we study the effect of temperature on molar volume of ZnO wurtzite type in the range of 300-3000K and 0-200GPa of temperature and pressure respectively. We analyze the relationship between pressure and temperature on molar volume; our data are in agreement with available results, although no more work under the previous conditions of pressure and temperature. Our work is very important in medicine, pharmacy, and geophysics, which need confirmation in future. of temperature and pressure respectively. We analyze the relationship between pressure and temperature on molar volume; our data are in agreement with available results, although no more work under the previous conditions of pressure and temperature. Our work is very important in medicine, pharmacy, and geophysics, which need confirmation in future.

## Biography:

Yahia CHERGUI has completed his PhD from Badji Mokhtar University in Annaba, Algeria. He is a teacher in Boumerdes University since 2012. He has published more than 7 papers in reputed journals and has been serving as a referee with condensed matter journal (IOP) and Energy journal (Elsevier). He passed 6 months in Cardiff University and Queen University for summer school.

## Recent Publications:

1) - N. Nehaoua, Y. CHERGUI and D. E. Mekki Tandem and single organic solar cells parameters evaluation from illumination IV plot Journal of Electron Devices, Vol. 11, 2011, pp. 515-520



- 2)- N.Nehaoua, Y. CHERGUI and D. E. Mekki. Determination of organic solar cell parameters based on single or multiple pin structures, Vacuum 84 (2010) 326-329.
- 3) - Y. CHERGUI, N. Nehaoua and D. E. Mekki. The structural properties of PbF2 by Molecular Dynamics Eur. Phys. J. Appl. Phys. 51, 20502 (2010). DIO:10.1051/epjap/2010096
- 4) - Y. CHERGUI, N. Nehaoua and D. E. Mekki Chapitre 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: parameters evaluation,
- 5) - N. Nehaoua, Y. CHERGUI and D. E. MEKKI Chapitre Solar Cells / Book 3 (first edition July 2011, InTec), ISBN 9-953-307-192-2