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Zinc Oxide Properties Under Different Conditions of Pressure and Temperatures a Molecular Dynamics Simulation

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Abstract

Zinc oxide semiconductor is a promised material due to its properties between ionic and covalent band. In this work we investigate molecular dynamics and dl_poly_4 software to analyze the band behavior under the effect of pressures and temperatures. Our system composed of 2916 atoms in a simulation box of 9x9x9 dimension. The range of pressure is 0-200GPa and for temperature is 300-3000K, we will study the variation of the distance between ZnO atoms. Our results are in agreement with the available data due to no more information under previous conditions. This result is very important in nanosacle and macroscale especially in industry field and geophysics.

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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 (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.