1er Congrès National de Physique et Chimie Quantique, "CPCQ 2015", Université Mouloud Mammeri , Tizi-Ouzou, 31/03 au 02/ 04/ 2015

2015

Theoretical investigation of optical properties of zinc blende III-Antimony materials

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Abstract : A first-principles calculations have been performed, using the Full Potential Linearized Augmented Plane Wave (FP-LAPW) calculations based on Density Functional Theory (DFT) method as implemented in Wien2k code, to evaluate the optical properties of III-Antimony binary compounds AlSb, GaSb and InSb, using the new semi-local modified Becke–Johnson potential (TB-mBJ) developed by Tran and Blaha. The real and the imaginary parts of the dielectric function, absorption coefficient, reflectivity and optical conductivity versus photon energy were presented to discuss optical properties of III-Sb. The results obtained were compared with experimental data and other computational works, suggesting our compounds as suitable materials for optoelectronic device applications.

Keywords : FP-LAPW, DFT, mBJ-BT, Optical parameters.