World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:17, No:11, 2023

Physical Properties of New Perovskite Kgex3 (X = F, Cl and Br) for Photovoltaic Applications

Authors : B. Bouadjemia, M. Houaria, S. Haida, Y. B. Idriss, A, Akham, M. Matouguia, A. Gasmia, T. Lantria, S. Bentataa

Abstract : It have investigated the structural, optoelectronic, elastic and thermodynamic properties of $KGeX_3$ (X = F, Cl and Br) using the density functional theory (DFT) with generalized gradient approximation (GGA) for potential exchange correlation. The modified Becke-Johnson (mBJ-GGA) potential approximation is also used for calculating the optoelectronic properties of the material.The results show that the band structure of the metalloid halide perovskites $KGeX_3$ (X = F, Cl and Br) have a semiconductor behavior with direct band gap at R-R direction, the gap energy values for each compound as following: 2.83, 1.27 and 0.79eV respectively. The optical properties, such as real and imaginary parts of the dielectric functions, refractive index, reflectivity and absorption coefficient, are investigated. As results, these compounds are competent candidates for optoelectronic and photovoltaic devices in this range of the energy spectrum.

Keywords : density functional theory (DFT), semiconductor behavior, metalloid halide perovskites, optical propertie and photovoltaic devices
Conference Title : ICNED 2023 : International Conference on Nanoelectronics Engineering and Devices
Conference Location : Jeddah, Saudi Arabia
Conference Dates : November 20-21, 2023