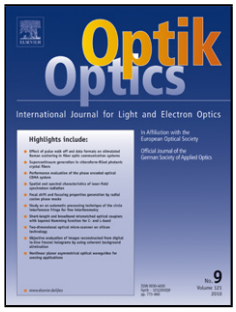

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An insight into electronic and optical properties of the chalcopyrite $CuGaSe_2$ compound under low pressure, calculations from mBJ potential and topological analysis of electron density

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Abstract

In this study, we pay attention to electronic, bonding and optical properties of the $CuGaSe_2$ compound as well as in the absence and under the application of hydrostatic pressure. We conducted this study within the approach of first principles calculations based on density functional theory. Our work yielding within the mBJ potential and other approximations, provide an improved theoretical prediction of both energy band gap value and optical quantities. In addition, results based topological partition of electron density give an adequate bonding description of both bonds and related dipolar momentums. The study provides also analysis of the investigated properties under pressure. We found that the pressure promotes the use of the $CuGaSe_2$ compound for more photovoltaic applications.

Keywords: $CuGaSe_2$; Pressure applied; mBJ potential; Electronic structures; Optical properties; Bonding properties