The Possible integration of the Double Perovskite Ba_2XSbO_6 (X=Sc,In) Compounds in solar cells technologies

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Abstract: In this work, we have comprehensively investigated DFT investigation on optoelectronic, properties of Ba_2InSbO_6 and Ba_2ScSbO_6 double perovskite oxides. The structural optimization was carried out using generalized gradient approximation (PBEsol-GGA). Moreover, the new Becke-Johnson (new-mBJ) was utilized in the framework of PBEsol GGA to precisely evaluate the electronic bandgaps. the material demonstrates a direct bandgap of 1.62 eV and 4.02 eV for Ba_2InSbO_6 and Ba_2ScSbO_6 respectively. Based on these bandgap values and the optic properties, the studied materials illustrate different properties, signifying different possible applications. Specially for solar cell technologies and light emitting elements.

Keywords: Perovskites, Solar cell, Energy.