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STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF $BaSnA_3$ (A=S or Se); A DFT study

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Abstract – Chalcogenide perovskites play an important role in the solar cell photovoltaic applications. A lot of researches in the present decade studied these materials, such as optical and photo-electric properties. Herein we are applied first principles density functional theory (DFT) to study the structural, electronic and optical properties of $BaSnS_3$ and $BaSnSe_3$ compounds. Gradient generalized approximations GGA-PBE and GGA-WC from the DFT was implemented in CASTEP (Cambridge Serial Total Energy Package) and used in our calculations. Results indicated that both $BaSnS_3$ and $BaSnSe_3$ crystallize in the orthorhombic structure and have a semi-conductivity behavior with energy gap between 0,35 eV and 0,97 eV. This paper prospects more works in the perovskites based-Sn.

Keywords – Chalcogenide Perovskites, $Basns_3$, $Basnse_3$, DFT, Semi-Conductivity Behavior.