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Lead-free semiconductors with high absorption: insight into the optical properties of $K_2GeSnBr_6$ and K_2GeSnI_6 halide double perovskites

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In this study, using the first-principles calculations, we have applied the full potential linearized augmented plane wave (FP-LAPW) method based on density functional theory (DFT) implemented in the code wien2k to study structural, electronic and optical properties of two halide double perovskites: $K_2GeSnBr_6$ and K_2GeSnI_6. The approximations used are generalized gradient approximation (GGA) and for exchange and correlation potential, we have applied a modified version of the potential proposed by Becke–Johnson (mBJ) to our compounds in order to improve the bandgaps and approach them to the experimental results.

Structural properties show that these two compounds are cubic and that they crystallize in the space group (Fm-3m, # 225), they also present a NM phase (non magnetic phase) which has the lowest energy compared to ferromagnetic and antiferromagnetic phases. The study of electronic properties is divided in two parts: the first one is for the band structure. The results show that these two compounds present a semiconductor behavior with direct band gap. The second one is for total and partial density of States. Results presented here confirm the semiconductor behavior observed in the band structure with a high impact of *s*-orbital of Sn and *p*-orbital of Br for valence band, while for conduction band there is a predominance of hybridization between *p*-orbital of Sn and *p*-orbital of metalloids used.

The most important parameter for optical properties is the dielectric function which has real and imaginary parts. The results obtained show that these compounds are suitable for storing sun light due to high values of absorption coefficient and that they are also reflective in optical devices.

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