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Ab Initio Study of Hexahalometallate Single Crystals K2XBr6 (X=Se, Pt)

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Abstract : Some physical properties of hexahalometallate $K_2XBr_6(X=Se,Pt)$ were computed in the zinc blend structure using generalized gradient approximation. The cell constant of K_2SeBr_6 and K_2PtBr_6 is consistent with the experiment value quoted in the literature, where the error is 0.95 % and 1 %. K_2SeBr_6 and K_2PtBr_6 present covalent bonding, high anisotropy and are ductile. The elastic constants of K_2SeBr_6 and K_2PtBr_6 are significantly smaller due to their larger reticular distances and lower Colombian forces, and then they are soft and damage tolerant. The interatomic separation is greater in K_2SeBr_6 than in K_2PtBr_6 ; hence the Colombian interaction in K_2PtBr_6 is greater than that of K_2SeBr_6 . The internal coordinate of the Br atom in K_2PtBr_6 is lower than that of the same atom in K_2SeBr_6 , and this can be explained by the fact that it is inversely proportional to the atom radius of Se and Pt. There are two major plasmonic processes, with intensities of 3.7 and 1.35, located around 53.5 nm and 72.8 nm for K_2SeBr_6 and K_2PtBr_6 .

Keywords: hexahalometallate, band structure, morphology, absorption, band gap, absorber

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