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# Ab Initio Study of Hexahalometallate Single Crystals $K_2XBr_6$ (X=Se, Pt)

**Authors :** M. Fatmi, B. Gueridi, Z. Zerrougui

**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 $K2SeBr_6$. The internal coordinate of the Br atom in $K_2PtBr_6$ is lower than that of the same atom in $K2SeBr_6$, 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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