Ab-initio Study of structural, elastic, electronic and optical properties of hexahalometallate single crystals $\text{K}_2\text{XBr}_6 (\text{X} = \text{Se}, \text{Pt})$

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Some physical properties of hexahalometallate $\text{K}_2\text{XBr}_6 (\text{X} = \text{Se}, \text{Pt})$ were computed in the zinc blend structure using GGA-PBESOL. The cell constant of $\text{K}_2\text{SeBr}_6$ and $\text{K}_2\text{PtBr}_6$ is consistent to the experiment value quoted in the literature, where the error is 0.95% and 1%. $\text{K}_2\text{SeBr}_6$ and $\text{K}_2\text{PtBr}_6$ present covalent bonding, high anisotropy and are ductile. The elastic constants of $\text{K}_2\text{SeBr}_6$ and $\text{K}_2\text{PtBr}_6$ are significantly smaller due to their larger reticular distances, lower Coulomb forces and then they are soft and damage tolerant. The interatomic separation is greater in $\text{K}_2\text{SeBr}_6$ than in $\text{K}_2\text{PtBr}_6$, hence the Coulomb interaction in $\text{K}_2\text{PtBr}_6$ is greater than that of $\text{K}_2\text{SeBr}_6$. The internal coordinate of Br atom in $\text{K}_2\text{PtBr}_6$ is lower than that of the same atom in $\text{K}_2\text{SeBr}_6$, 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 3.7 and 1.35 located around 53.5 nm and 72.8 nm for $\text{K}_2\text{SeBr}_6$ and $\text{K}_2\text{PtBr}_6$.

Progress in experiment and theory, coupled with computational model is accelerating the discovery of new materials with useful physical parameters. The cubic antifluorite class $\text{K}_2\text{XBr}_6 (\text{X} = \text{Pt}, \text{Se})$ have received increased interest since they exhibit structural phase transitions at lower temperatures. The family of hexahalometallate attracts researchers due to their light-absorbing materials in photovoltaic applications. The hexahalometallate double perovskites $\text{K}_2\text{XBr}_6 (\text{X} = \text{Pt, Se})$ crystallize in the cubic antifluorite $\text{K}_2\text{PtCl}_6$ structure. They have the stoichiometric formula $\text{X}_2\text{MA}_6$, where X, M and A are alkaline metal, polyvalent or heavy transition metal and halogen. The K atom in $\text{K}_2\text{XBr}_6 (\text{X} = \text{Pt, Se})$ of the three-dimensional structure is bonded to twelve equivalents Br atoms to form $\text{KBr}_{12}$ cuboctahedra. The faces contain six equivalents $\text{KBr}_{12}$ cuboctahedra and four equivalents $\text{PtBr}_6$ ($\text{SeBr}_6$) octahedral. Studies conducted by other researchers, it is stated that, the investigation on elastic constants and compressibility of $\text{K}_2\text{XBr}_6 (\text{X} = \text{Pt, Se})$ has carried out experimentally by N. Wruk et al. using Brillouin scattering and ultrasonic wave velocity measurements¹. The study conducted by Walter Abriel and Mary Anne White on $\text{K}_2\text{SeBr}_6$ by x-ray powder diffraction in the temperature range 10 K to 290 K, and heat capacity measurements indicates three phases for $\text{K}_2\text{SeBr}_6$, $\text{K}_2\text{PtCl}_6$ cubic structure, $\text{Rb}_2\text{TeI}_6$ tetragonal structure and $\text{K}_2\text{TeBr}_6$ monoclinic structure². The phase-transition temperatures of hexahalometallate material $\text{K}_2\text{PtBr}_6$ ($\text{K}_2\text{SeBr}_6$) have been studied experimentally and found to be 209 K, 221 K and 249 K¹ (78 K, 105 K, 137 K, 143 K and 169 K). $\text{K}_2\text{XBr}_6 (\text{X} = \text{Pt, Se})$ hexahalometallate materials show a suitable energy gap, sufficient absorption, low reflectivity, weaker cost and therefore adequate performance for photovoltaic applications²,³. Our study confirms the characteristics of mentioned materials above, which have a band gap range of (0.98 eV to 2.25 eV), an absorption coefficient of 237,311 cm⁻¹ (211,556 cm⁻¹) and reflectivity of (0.1–0.3%) in the extreme ultraviolet light. The band gap range (1–2.25 eV) and the absorption of extreme ultraviolet light make $\text{K}_2\text{SeBr}_6$ and $\text{K}_2\text{PtBr}_6$ as absorber materials in solar cells. These compounds are poor reflector and can be used as an anti-reflection coating material.

The aim of this work is the use of GGA-PBESOL and HSE hybrid approximations to obtain adequate structural, elastic and optoelectronic properties of $\text{K}_2\text{XBr}_6 (\text{X} = \text{Pt, Se})$. The paper is organized such as the calculation

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Calculation scheme
Calculations were carried out using the DFT framework as implemented in the CASTEP code. The valence states of K₂XBr₆ (X = Se, Pt) are K: 4s¹, Se: 4p⁴, Pt: 5d⁹ and Br: 4p⁵. An ultra soft pseudo-potential type Vanderbilt describes the interaction of valence electrons and ions cores. The GGA-PBESOL of Perdew et al. is adopted for the non-local correlation exchange effect. The best convergence of the computed structures and energies requires the use of cut-off energy of 630 eV. The irreducible Brillouin zone was sampled up to 8 × 8 × 8 k-grid on the Monkhorst–Pack scheme. The tolerance of geometry optimization were a difference of total energy 5 × 10⁻⁶ eV/atom, a maximum ionic Hellmann–Feynman force 10⁻² eV/Å, maximum stress 2 × 10⁻² eV/Å³ and ionic displacement of 5 × 10⁻⁴ Å. The calculation of the optical parameters requires the use of uniform distribution of 20 × 20 × 20 k-points. The self-consistent calculations converge if the total energy is minimal. The structural parameters were estimated using the minimization technique of Broyden-Fletcher-Goldfarb-Shanno (BFGS), which provide a fast way to find the lowest energy structure. The basic idea behind the hybrid functionals is to mix exchange energies calculated in an exact (Hartree–Fock-like) manner with those obtained from DFT methods in order to improve performance. The accuracy of the electronic properties predicted by density functional theory depends on the used exchange–correlation functional. Non-local hybrid functionals gives more accurate results than semi-local functionals. The non-local Hartree–Fock exchange is an integral part of the hybrid functionals implemented in the FLAPW method. The non-local exchange in HSE enlarges the elements of the optical transition matrix and leads to better accuracy of HSE in calculating electronic properties. Omitting the non-local exchange in the transition operator for HSE leads to errors. The importance of non-local correction in the velocity gauge has been widely discussed for non-local pseudo potentials. The non-locality of the potential comes from the fact that the electron Hamiltonian is replaced by an approximate Hamiltonian in the independent electron approximation with an effective potential, which reintroduces the electron–electron interactions in the Kohn–Sham equations.

Results and discussion
Structure and morphology. The crystal structure of K₂PtBr₆ is illustrated in Fig. 1. The location of atoms is such that (Se, Pt) atom is placed at the center of the octahedron formed by the four atoms of Br. The K atoms occupy interstitial sites. The antifluorite class K₂XBr₆ (X = Se, Pt) adopt the cubic structure with space group Fm3m at ambient conditions. The occupied Wyckoff sites for K, (Se, Pt) and Br atoms are ± (1/4, 1/4, 1/4) a₀, (0, 0, 0) a₀ and ± (x, 0, 0) a₀, ± (0, x, 0) a₀, ± (0, 0, x) a₀. The lattice constant, bulk modulus and its pressure derivative of K₂XBr₆ (X = Se, Pt) are listed in Table 1. The cell constant of K₂SeBr₆ and K₂PtBr₆ is consistent to the experimental value quoted in the literature, where the error is 0.95% and 1%. The bulk modulus calculated for K₂SeBr₆ and K₂PtBr₆ using the fit scheme P(V/V₀) as reported in Fig. 2 is in good agreement with available experimental data. The interatomic distances dX-Br, dK-Br and dBr-Br in K₂SeBr₆ (K₂PtBr₆) at equilibrium are 2.5681 Å, 3.6769 Å and 3.6319 Å (2.4703 Å, 3.6306 Å and 3.4936 Å). It should be pointed that, bond lengths reported for K₂SeBr₆ are in good agreement with those found in the literature dSe-Br = 2.555 Å, dBr-Se = 2.50 Å, dK-Br = 3.685 Å and dBr-Br = 3.613 Å. Figure 3 shows the effect of pressure on dK-Br, dBr-Br and dBr-X (X = Se, Pt) bond lengths in K₂SeBr₆ and K₂PtBr₆. The bond lengths in K₂SeBr₆ are larger than those in K₂PtBr₆, hence, the
Coulomb interaction in K2PtBr6 is greater than that in K2SeBr6, which can be explained by the fact that the distances are inversely proportional to the lattice constant. Also, the distance d_{Br-Se} is greater than that of d_{Br-Pt}. All bond lengths decrease monotonously when the pressure increases. Figure 4 displays the effect of pressure on the internal coordinate of Br atom in K2SeBr6 and K2PtBr6. The internal coordinate of Br atom in K2PtBr6 is lower than that of the same atom in K2SeBr6, and this is explained by the fact that it is inversely proportional to the atom radius of Se (1.15 Å) and Pt (1.35 Å).

Table 1. The lattice constant, bulk modulus and its pressure derivative and elastic moduli of K2XBr6 (X = Se, Pt).

|                  | K2SeBr6 | K2PtBr6 |
|------------------|---------|---------|
|                  | This Work | Experiment | Other |
| A (Å)            | 10.265  | 10.363 i | 10.3995 | 10.293 i |
| x                | 0.24065 | 0.24695 |
| B0 (GPa)         | 15.35   | 16.70 i | 15.43 | 15.20 i |
| B'               | 6.15    | 7.20    |
| C_{11} (GPa)     | 15.49   | 23.20 i | 22.27 | 21.60 i |
| C_{12} (GPa)     | 11.95   | 13.50 i | 8.97 | 12.0 i |
| C_{44} (GPa)     | 7.08    | 9.30 i  | 5.95 | 8.50 i |

Figure 2. The pressure effect on normalized volume in K2SeBr6 and K2PtBr6.
Elastic constants and related parameters. The knowledge of elastic constants is essential for a better theoretical understanding of the properties of materials that are determined by the phonons density of states and the electron–phonon interaction processes. The three independent elastic constants $C_{11}$, $C_{12}$ and $C_{44}$ require for their elastic characterization. The elastic moduli of $K_2XBr_6 (X = \text{Se, Pt})$ computed at equilibrium using GGA-PBESOL are reported in Table 1. No theoretical value is reported in the literature, then our computation is prediction. The elastic constants of $K_2\text{SeBr}_6$ and $K_2\text{PtBr}_6$ are significantly small because of their quite large reticular distances, low Colombian forces, so they are quite soft and tolerant to damage. This result is qualitatively explained in these two materials by their binding forces, which are mainly ionic. It was noted that $C_{11}$, $C_{12}$ and $C_{44}$ agree reasonably with their experiment values\(^1\). The elastic stability of $K_2\text{SeBr}_6$ and $K_2\text{PtBr}_6$ was defined taking into account the Born's criteria, from which the following conditions must be satisfied for zinc blend structure\(^18\):

$$\sigma(C_{11} + 2C_{12}) = 0, \sigma(C_{44}) = 0, \sigma(C_{11} - C_{12}) = C_{12}(C_{11})$$ (1)

The bulk modulus calculated from the elastic constants is identical to that deduced from equation of state fitting $P(V/V_0)$. This makes our results as reliable. Figure 5 visualizes the dependence on pressure of $K_2XBr_6 (X = \text{Se, Pt})$ elastic moduli. It is observed that the elastic values of GGA-PBESOL increase as a function of the applied
pressure, from zero to 20 GPa. These compounds show weaker elastic constants, which explain their lower hardness. The bulk modulus, shear modulus, Young's modulus, Poisson's ratio, the universal anisotropy and $\frac{B_H}{G_H}$ ratio for isotropic polycrystalline materials of $K_2XBr_6 (X = Pt, Se)$ using the Voigt-Reuss-Hill approximation are reported in Table 2. The values of the Poisson coefficient between 0.25 and 0.5 are associated with the interatomic forces of central types and covalent bonding character. The nature of the bonds in a compound is described by the factor $\sigma$, either ionic-covalent ($0.16 \leq \sigma \leq 0.30$) in $K_2PtBr_6$ (0.29) and metallic ($\sigma \geq 0.33$) in $K_2SeBr_6$ (0.35). The Pugh's criterion ($\frac{B_H}{G_H}$) and universal anisotropy indicate that $K_2XBr_6 (X = Pt, Se)$ are ductile and anisotropic. The extreme values of Young's modulus, linear compressibility, shear modulus and Poisson's ratio for $K_2XBr_6 (X = Pt, Se)$ are listed in Table 3. These values prove the isotropic linear compressibility and confirm the anisotropy of the other parameters and the anisotropy is more pronounced in $K_2SeBr_6$. We represent in Fig. 6 using ELATE software the effect of orientation on mechanical parameters for $K_2PtBr_6$.

**Table 2.** The extreme values of Young's modulus (GPa), linear compressibility (GPa), shear modulus (GPa) and Poisson's ratio for $K_2XBr_6 (X = Pt, Se)$.

| Material   | Young's modulus $E_{\text{min}}$ | Linear compressibility $\beta_{\text{min}}$ | Shear modulus $G_{\text{min}}$ | Poisson's ratio $\sigma_{\text{min}}$ | Young's modulus $E_{\text{max}}$ | Linear compressibility $\beta_{\text{max}}$ | Shear modulus $G_{\text{max}}$ | Poisson's ratio $\sigma_{\text{max}}$ |
|------------|---------------------------------|-------------------------------------------|---------------------------------|-------------------------------------|---------------------------------|-------------------------------------------|---------------------------------|-------------------------------------|
| $K_2SeBr_6$ | 5.0801                          | 18.014                                    | 25.374                          | 7.0839                              | 15.565                          | 24.857                                    | 6.6484                          | 0.33683                             |
| $K_2PtBr_6$ | 15.565                          | 17.117                                    | 24.857                          | 5.9567                              | 18.014                          | 25.374                                    | 7.0839                          | 0.22305                             |

**Figure 5.** Elastic moduli of $K_2SeBr_6$ and $K_2PtBr_6$.

**Band structure and states densities.** Understanding the band structure and estimating band gap of $K_2XBr_6 (X = Pt, Se)$, we use both GGA (PBE-SOL) and HSE hybrid functional as shown in Fig. 7. The calcula-
tions were conducted on $K_2XBr_6$ ($X = Pt, Se$), by neglecting the presence of the K-state in the (Pt, Se) site. The electronic band structure of $K_2SeBr_6$ and $K_2PtBr_6$ were computed using the equilibrium lattice constant. The bottom of the conduction band is at $\Gamma$ point for $K_2SeBr_6$ and $K_2PtBr_6$. The top of the valence band is at $L$ and $X$ points in $K_2SeBr_6$ and $K_2PtBr_6$ compounds, which indicate an indirect band gap $\Gamma-L$ ($\Gamma-X$) of 1.5089 eV and 2.250 eV (0.9818 eV and 1.531 eV) for $K_2SeBr_6$ ($K_2PtBr_6$). No experimental and theoretical value are present in the literature, and then our results are predictions. Note that the HSE approximation gives a value close to the experimental one. We report the various band gaps at equilibrium lattice constant for $K_2SeBr_6$ and $K_2PtBr_6$ using GGA and HSE in Table 4. By varying the applied pressure between 0 and 20 GPa, the fundamental band gap as shown in Fig. 8 decreases. $K_2PtBr_6$ becomes metallic at a pressure of 15 GPa. We visualize the plots of PDOS and TDOS of $K_2SeBr_6$ and $K_2PtBr_6$ in Fig. 9. The top of valence band region is $-2.86$ eV to $E_F$ ($-2$ eV to $E_F$) for $K_2SeBr_6$ ($K_2PtBr_6$). The electronic contribution in this region is due mainly to Br: $p$ orbital in $K_2SeBr_6$ and $K_2PtBr_6$. The first conduction band of $K_2SeBr_6$ ($K_2PtBr_6$) starts at 1.68 eV (4 eV), then the transitions occur between Br: $p$ and K: $p$ sites. It is noted that the Pt site does not participate in the electronic contribution at the conduction and valence bands.

| Material   | B$_H$ (GPa) | B$_V$ (GPa) | G$_V$ (GPa) | G$_H$ (GPa) | $E_H$ (GPa) | $\sigma_H$ | $\lambda_H$ | $B_H/G_H$ |
|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-----------|
| $K_2SeBr_6$ | 13.137      | 13.137      | 13.137      | 4.9581      | 3.2179      | 4.088       | 11.111      | 0.35903   |
| $K_2PtBr_6$ | 13.41       | 13.41       | 13.41       | 6.2334      | 6.2154      | 6.2244      | 16.171      | 0.29902   |

Table 3. The bulk modulus, shear modulus, Young's modulus, Poisson's ratio, anisotropy factor and $B_H/G_H$ ratio for $K_2XBr_6$ ($X = Pt, Se$).

Figure 6. The orientation effect on Poisson's ratio, Young's modulus, linear compressibility and shear modulus in $K_2PtBr_6$. 
Figure 7. Band structures of $K_2XBr_6 (X = \text{Pt, Se})$ in zinc blend structure performed with GGA (PBE-SOL) and HSE hybrid.

| Material      | $E_{\text{g}}$ (eV) | $\alpha \times 10^{-2}$ (eV/GPa) | $\beta \times 10^{-3}$ (eV/GPa^2) |
|---------------|----------------------|----------------------------------|----------------------------------|
| $K_2\text{PBr}_6$ | 2.323                | 0.98                             | 1.88                             |
| $K_2\text{PtBr}_6$ | 2.56                 | 1.5                              | 1.902                            |
| $K_2\text{SeBr}_6$ | 2.29                 | 2.56                             | 2.58                             |
| $K_2\text{PtBr}_6$ | 2.58                 | 2.56                             | 1.56                             |

Table 4. The various band gaps at zero pressure for $K_2\text{SeBr}_6$ and $K_2\text{PtBr}_6$. 
Optical properties. The real dielectric constant is a measure of polarization, while the imaginary part is a measure of the dielectric losses. The complex dielectric function is the sum of real and imaginary parts.

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

The optical quantities such as reflectivity, absorption, loss function and refractive index depend on the structure of the material. These parameters cited above are isotropic in a material with cubic structure. The reflectivity of any material is calculated by dielectric function through the equation:

$$R(\omega) = \left| \frac{(\varepsilon_1)^{1/2} - 1}{(\varepsilon_1)^{1/2} + 1} \right|$$

We display the plots of reflectivity, absorption and loss function as a function of wavelength for K$_2$SeBr$_6$ and K$_2$PtBr$_6$ in Fig. 10. The reflectivity is a measure of the ability of a material to reflect radiation. The reflectivity of K$_2$SeBr$_6$ and K$_2$PtBr$_6$ starts at wavelength around 60 nm and reaches several peaks of maxima (0.23) and minima (0.05) in the field of extreme ultraviolet light. In practice, the roughness, uniformity of thickness, inter diffusion, oxidation and thermal stability limit the reflectivity. We observe various absorption peaks in extreme ultraviolet light. These peaks are due to the electronic transitions from the top of the valence band to the bottom of the conduction band. The maximum absorption is between 234,720 cm$^{-1}$ and 229,405 cm$^{-1}$ at wavelength range 56 nm to 105 nm for K$_2$SeBr$_6$ and K$_2$PtBr$_6$. Indeed, K$_2$SeBr$_6$ and K$_2$PtBr$_6$ have a narrow gap and absorb extreme ultraviolet light and consequently, they are candidates in the fields of photocatalysis and photovoltaic. The loss function is calculated through the equation:

$$L(\omega) = \frac{\varepsilon_2(\omega)}{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}$$

The loss function demonstrates the existence of two major plasmonic processes, with intensity 3.7 and 1.35 located around 53.5 nm and 72.8 nm. There is no loss in the ultra violet and visible light domains. We present in Fig. 11 the refractive index of K$_2$SeBr$_6$ and K$_2$PtBr$_6$ as a function of energy. The static refractive index is 2.583 (2.407) for K$_2$SeBr$_6$ (K$_2$PtBr$_6$). It reaches a series of maxima 3.106 (2.678) and minima 0.383 (0.485) between 1.7 eV and 23 eV for K$_2$SeBr$_6$ (K$_2$PtBr$_6$). It is reported that an experimental refractive index 2.15 and 2.11 for K$_2$SeBr$_6$ and K$_2$PtBr$_6$ calculated by N. Wruk et al. The refractive index is given as:

$$n(\omega) = \frac{\sqrt{\varepsilon_2}}{2} \left[ \varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2} \right]$$

The refractive index is more important when photons move through the material and when bonds between atoms are covalent. The static refractive index enhanced with the expansion of the electronic cloud and the increase in density on the structure. The general trend is that the decrease in reflectivity results from the increase...
in absorption and the decrease in refractive index. The plots of imaginary part and $E(k) = E_C(k) - E_V(k)$ for $K_2\text{SeBr}_6(X = \text{Se, Pt})$ are reported in Fig. 12 (right and left panel). The imaginary part and optical transitions are connected to the absorption coefficient. The main contribution to the optical transitions from six top valence bands to seven lower conduction bands for $K_2\text{SeBr}_6(X = \text{Se, Pt})$ are reported in Table 5. The isotropic optical parameters of $K_2\text{SeBr}_6$ and $K_2\text{PtBr}_6$ makes them as windows and lenses. The band gap range (1–2.25 eV) and absorption of extreme ultraviolet light make $K_2\text{SeBr}_6$ and $K_2\text{PtBr}_6$ as absorber materials.

**Conclusion**

Employing a plane-wave pseudo-potential using the DFT framework, within the generalized gradient approximation, we studied the structural, mechanical and optoelectronic parameters of $K_2\text{PtBr}_6$ and $K_2\text{SeBr}_6$ hexahalometallate materials. The bulk modulus of $K_2\text{SeBr}_6$ and $K_2\text{PtBr}_6$ agrees well with experiment value where the error
is 8% and 1.4%. The elastic constants of K$_2$SeBr$_6$ and K$_2$PtBr$_6$ are significantly smaller, then they are fairly soft and damage tolerant. An electronic study shows that K$_2$PtBr$_6$ is indirect band gap semiconductor and becomes metallic at a pressure of 15 GPa. The partial density of states indicates that the valence electrons are transferred from Br: p state to K: p site. The band gap size, optical absorption and reflectivity make K$_2$SeBr$_6$ and K$_2$PtBr$_6$ as candidate absorbers. The static refractive index increases with the expansion of the electronic cloud and the increase in density on the structure. The general trend is that the decrease in reflectivity results from the increase in absorption and the decrease in refractive index. There is no loss in the ultra violet and visible light domains. The compounds are poor reflector and can be used as an anti-reflection coating material.

Figure 10. The reflectivity, absorption and loss function in K$_2$SeBr$_6$ and K$_2$PtBr$_6$.

Figure 11. The refractive index in K$_2$SeBr$_6$ and K$_2$PtBr$_6$.
Figure 12. The imaginary part and transition energy in K₂SeBr₆ and K₂PtBr₆.
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Competing interests

The authors declare no competing interests.

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