**Ab-initio** calculations on structural, electronic, half-metallic and optical properties of Co-, Fe-, Mn- and Cr-doped Ba$_2$LuTaO$_6$

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Abstract. Full potential-linearised augmented plane wave (FP-LAPW) method is used to study the structural, electronic, half-metallic and optical properties of Ba$_2$LuTaO$_6$ doped with d-block atoms Co, Fe, Mn and Cr using density functional theory (DFT) technique. Ba$_2$LuTa$_{0.75}$TM$_{0.25}$O$_6$ supercells were constructed by doping 3d transition metal atoms Co, Fe, Mn and Cr with 2.5% of concentration in Ba$_2$LuTaO$_6$ host compound. The possibility of half-metallic ferromagnetism in Ba$_2$LuTa$_{0.75}$TM$_{0.25}$O$_6$ (TM = Co, Fe, Mn and Cr) was analysed by electronic band structure and density of state calculations. We found that Ba$_2$LuTa$_{0.75}$(Co and Cr)$_{0.25}$O$_6$ alloys exhibit complete half-metallic characteristics with a total spin moment of 2.00 and 1.00 $\mu_B$ and direct band gap of $E_g^\uparrow = 0.52$ eV and $E_g^\downarrow = 1.60$ eV, respectively. These results may be of interest for spintronics applications. Moreover, the optical properties of the material in question are also examined and discussed.

Keywords. Ba$_2$LuTa$_{0.75}$TM$_{0.25}$O$_6$; magneto-optic; spintronics; ab-initio calculations.

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1. Introduction

Recently, double-perovskite compounds like A$_2$BB’O$_6$ attracted a great deal of attention because of their possible applications in numerous industrial and engineering fields [1–11]. New generation perovskites of double perovskites have attracted lots of attention because of their promising technological applications in photovoltaic, photodetector or photocatalytic fields [12–14].

Half-metallic materials are materials that act as conductors for electrons in one spin orientation, but as insulators or semiconductors for electrons in opposite spin orientation [15]. Generally, many half-metals are oxides or Heusler alloys [16,17]. These materials have attracted much attention due to their potential use in spintronics [18]. One of the promising applications of spintronics is in multiple-states memory devices, such as tunnelling magnetoresistance and giant magnetoresistance, whose functions totally depend on magnetisation and can only be realised by using spin direction [19].

Half-metallic ferromagnets represent a new class of materials which attract a lot of attention because of their possible applications in spintronics [20]. These materials have complete (100%) spin polarisation at the Fermi level because one spin channel is metallic while the other channel is semiconducting. Various half-metallic ferromagnetics, such as double perovskites (for example, CuMn$_2$InSe$_4$ [21] and UX$_2$O$_6$ [22], zinc blende (ZB) CaC and CaN compounds [23], suzuki-type compounds Li$_6$TMCI$_8$ [24], perovskite XAlO$_3$ (X = Cs, Rb and K) [25], quaternary Heusler compounds (for example, PtZrTiAl, PdZrTiAl, CoMn-CrSb and Ti$_2$RhSn$_{1−x}$Si$_x$) [26–28] have been predicted by the first-principles calculations or experimentally synthesised.

The electronic structure and magnetic properties of the Sr$_2$GdReO$_6$ double perovskite were investigated. The results indicate that this double perovskite may become an ideal candidate material for future spintronic applications [29]. In a very recent study, the structural, electronic and half-metallic properties of double perovskite RBaMn$_2$O$_{6−δ}$ (R = Nd, Pr, La and $δ = 0, 1$) compounds were studied, and the results show that they are half-metallic ferromagnets [30]. Furthermore, the Sr$_2$XOsO$_6$ (X = Cs, Rb and K) compounds have been investigated theoretically and half-metallicity is
found in all the three compounds. Elastic constants $C_{ij}$, shear modulus $G$, Young’s modulus $E$, Poisson ratio $\nu$, anisotropic factor $A$ and Cauchy’s pressure $C_{11}-C_{44}$ for the studied compounds were also calculated [31].

In this work, a new series of four Ba$_{2}$LuTa$_{0.75}$TM$_{0.25}$O$_{6}$ alloys are studied theoretically where TM is the main group element corresponding to Co, Fe, Mn and Cr. To our best knowledge, the studied Ba$_{2}$LuTa$_{0.75}$TM$_{0.25}$O$_{6}$ materials are not investigated earlier. We selected these materials because of the unavailability of any theoretical or experimental data for the Ba$_{2}$LuTa$_{0.75}$TM$_{0.25}$O$_{6}$ alloys in literature. In this paper, our efforts are focussed on simple yet robust first-principles calculations of the Ba$_{2}$LuTa$_{0.75}$TM$_{0.25}$O$_{6}$ alloys in terms of the structural, electronic, half-metallic and optical properties. The paper is arranged as follows: Section 1 gives introduction, the computational background will be discussed in §2, results are reported and discussed in §3 and a precise summary of the results is given in §4.

2. Method of calculation

As mentioned already, we have considered the experimental crystal parameters as reported by Galasso [32]. The calculations were based on the supercell (i.e., $1 \times 1 \times 1$) where one Ta atom at (0.5,0.5,0.5) in the positions in a cubic of the supercell approach of Ba$_{2}$TaLuO$_{6}$ is replaced by Co, Fe, Mn and Cr atoms, respectively. An elementary crystal structure containing 40 atoms was established. We found Ba$_{2}$Ta$_{0.75}$TM$_{0.25}$LuO$_{6}$ alloy thermodynamically stable in cubic symmetry of space group PM-3M (n°221). The crystal structures of Ba$_{2}$Ta$_{0.75}$TM$_{0.25}$LuO$_{6}$ alloy is shown in figure 1.

To compute the structural, electronic, optical and half-metallic properties of the Ba$_{2}$Ta$_{0.75}$TM$_{0.25}$LuO$_{6}$ alloys, we have applied the density functional theory (DFT)-based self-consistent cycle of full-potential linearised

Figure 1. Crystal structure of Ba$_{2}$LuTa$_{0.75}$TM$_{0.25}$O$_{6}$.

Figure 2. Calculated normalised energy as a function of volume for both pristine and doped Ba$_{2}$LuTaO$_{6}$ compound.
Table 1. Lattice constants $a$ (Å), bulk modulus $B$ (in GPa) and its bulk modulus pressure derivative $B'$. 

<table>
<thead>
<tr>
<th>Compounds</th>
<th>Method</th>
<th>Point group</th>
<th>Stat</th>
<th>$a$ (Å)</th>
<th>$B$ (GPa)</th>
<th>$B'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ba$_2$LuTaO$_6$</td>
<td>GGA + $U$</td>
<td>Fm-3m</td>
<td>FM</td>
<td>8.45</td>
<td>148.86</td>
<td>4.41</td>
</tr>
<tr>
<td></td>
<td>GGA + $U$</td>
<td>Fm-3m</td>
<td>PM</td>
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<td>149.07</td>
<td>4.47</td>
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<tr>
<td></td>
<td>EXP</td>
<td>Fm-3m</td>
<td>PM</td>
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<td>–</td>
<td></td>
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<tr>
<td></td>
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<td>Fm-3m</td>
<td>PM</td>
<td>8.3659 [41]</td>
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</tr>
<tr>
<td>EXP</td>
<td>Other</td>
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<td>PM</td>
<td>8.423 [42]</td>
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<td></td>
</tr>
<tr>
<td>Ba$<em>2$LuTa$</em>{0.75}$Co$_{0.25}$O$_6$</td>
<td>GGA + $U$</td>
<td>Pm-3m</td>
<td>FM</td>
<td>8.46</td>
<td>195.57</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>GGA + $U$</td>
<td>Pm-3m</td>
<td>PM</td>
<td>8.45</td>
<td>197.23</td>
<td>–</td>
</tr>
<tr>
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<td>FM</td>
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<tr>
<td></td>
<td>GGA + $U$</td>
<td>Pm-3m</td>
<td>PM</td>
<td>8.37</td>
<td>189.47</td>
<td>–</td>
</tr>
<tr>
<td>Ba$<em>2$LuTa$</em>{0.75}$Cr$_{0.25}$O$_6$</td>
<td>GGA + $U$</td>
<td>Pm-3m</td>
<td>FM</td>
<td>8.42</td>
<td>195.27</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>GGA + $U$</td>
<td>Pm-3m</td>
<td>PM</td>
<td>8.41</td>
<td>196.27</td>
<td>–</td>
</tr>
<tr>
<td>Ba$<em>2$LuTa$</em>{0.75}$Mn$_{0.25}$O$_6$</td>
<td>GGA + $U$</td>
<td>Pm-3m</td>
<td>FM</td>
<td>8.46</td>
<td>190.88</td>
<td>–</td>
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<tr>
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<td>GGA + $U$</td>
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<td>PM</td>
<td>8.44</td>
<td>196.27</td>
<td>–</td>
</tr>
</tbody>
</table>

Figure 3. Spin-polarised band structure and total densities of states (TDOS) for Ba$_2$LuTaO$_6$.

The exchange-correlation energy correction is parametrised by using the generalised gradient approximation (GGA) plus Hubbard $U$ term [35] which is surprisingly appropriate for the improved band gaps of solids compared to GGA and gives accurate values of the electronic band gaps close to the experimental ones. The region is divided into interior non-overlapping space between muffin-tin (MT) spheres and the interstitial region between these spheres. The spherical harmonic functions and Fourier series originated from a basis function are employed for MT spheres and interstitial regions, respectively. The 3d orbital of the transition metal atoms was treated using the GGA + $U$ approach with the values of $U_{\text{eff}}$ taken to be 6.88, 6.04, 5.91 and 4.97 eV for Co, Mn, Fe and Cr atoms similar to refs [36,37]. The mesh of $K$ points in the first Brillouin zone by the centre of $\Gamma$ point was selected as $12 \times 12 \times 12$. We have chosen $l_{\text{max}}, R_{\text{MT}} \rightarrow K_{\text{max}}$ and $G_{\text{max}}$ to be 10, 9 and 14, respectively. A dense $k$-mesh with 5000 $k$-points was used in the first Brillouin zone to calculate linear optical properties.
Optical properties of a solid are usually described in terms of the complex dielectric function \( \varepsilon(w) = \varepsilon_1(w) + i\varepsilon_2(w) \). The imaginary part \( \varepsilon_2(w) \) was calculated from the momentum matrix elements between the occupied and unoccupied wave functions within the selection rules. The real part \( \varepsilon_1(w) \) of the dielectric function was calculated by the Kramers–Kronig transformation \[38\] of the imaginary part \( \varepsilon_2(w) \). Optical constants such as refractive index \( n(w) \) and extinction coefficient \( k(w) \), are calculated in terms of the real and the imaginary parts of the complex dielectric function as follows \[39\]:

\[
n = \left( \varepsilon_1 + (\varepsilon_1^2 + \varepsilon_2^2)^{1/2} \right)^{1/2} / \sqrt{2}.
\]  

3. Results and discussion

Specifically, \( \text{Ba}_2\text{LuTaO}_6 \) and \( \text{Ba}_2\text{LuTa}_{0.75}\text{TM}_{0.25}\text{O}_6 \) crystallise in a cubic nested symmetrical crystal structure having symmetry groups \( \text{Fm}-3\text{m} \) and \( \text{Pm}-3\text{m} \), respectively. For the optimisation of the structure and geometry of the crystal, Birch Murnaghan’s equation \[40\] of state is used to find the total energy/unit cell at different volumes. The minimum ground-state energy is clearly visible by optimising the unit cell structure into FM (FM) and non-magnetic (NM) configurations within GGA+U functional scheme. Figure 2 clearly shows that the lowest energy corresponds to the FM phase rather than the NM phase and hence FM phase is thermodynamically more stable. Subsequently, several optimised structural parameters at ambient conditions, viz., lattice constant \( \text{in}\ \text{Å} \), bulk modulus \( (B) \) and its pressure derivative \( (B') \) are given in table 1. Also shown for comparison are the available experimental data from the literature. A good accord can be observed between our findings and the experimental and theoretical results reported in refs \[32,41,42\] regarding lattice parameters for the \( \text{Ba}_2\text{LuTaO}_6 \) compound.

Investigations of the electronic band structure and the density of states are important because most of

![Figure 4. Band structure for high-symmetry directions in the Brillouin zone for (a) \( \text{Ba}_2\text{LuTa}_{0.75}\text{Co}_{0.25}\text{O}_6 \), (b) \( \text{Ba}_2\text{LuTa}_{0.75}\text{Cr}_{0.25}\text{O}_6 \), (c) \( \text{Ba}_2\text{LuTa}_{0.75}\text{Fe}_{0.25}\text{O}_6 \) and (d) \( \text{Ba}_2\text{LuTa}_{0.75}\text{Mn}_{0.25}\text{O}_6 \).]
the physical properties of solids are related to them. The self-consistent scalar relativistic band structures as well as total density of states for pure and doped Ba$_2$LuTaO$_6$ along various symmetry lines are given in figures 3–6. Figure 3 shows band structure and total density of state (TDOS) of pure Ba$_2$LuTaO$_6$. Note that there is a wide band gap around the Fermi level. The band gap value is determined and found to be 3.42 eV (see table 2). This indicates that the undoped Ba$_2$LuTaO$_6$ has a wide band gap semiconductor character. For the Ba$_2$LuTaO$_6$ compound, both the valence band maximum (VBM) and conduction band minimum (CBM) occur at the high-symmetry point $\Gamma$ in the Brillouin zone. This suggests that the material under load is a direct ($\Gamma$-$\Gamma$) band-gap semiconductor. This is consistent with the theoretical findings reported in ref. [41]. Figures 3 and 4 represent the electronic band structures and TDOS and partial density of states (PDOS) of doped materials of interest. We remark from TDOS of the compounds Ba$_2$LuTa$_{0.75}$Cr$_{0.25}$O$_6$ and Ba$_2$LuTa$_{0.75}$Co$_{0.25}$O$_6$ that they are half-metallic materials. The half-metallic band gap is found in spin-down state (minority) for Ba$_2$LuTa$_{0.75}$Cr$_{0.25}$O$_6$. Nevertheless, for Ba$_2$LuTa$_{0.75}$Co$_{0.25}$O$_6$, the band gap is seen in spin-up state (majority). The magnitudes of these band gaps are calculated and found to be $E_g \downarrow = 1.60$ eV and $E_g \uparrow = 0.52$ eV for Ba$_2$LuTa$_{0.75}$Cr$_{0.25}$O$_6$ and Ba$_2$LuTa$_{0.75}$Co$_{0.25}$O$_6$, respectively. It is observed that the doping of 3d transition metal atoms causes a change in the energy band gap as clearly seen in the band structure of the new Ba$_2$LuTa$_{0.75}$ (Cr and Co)$_{0.25}$O$_6$ materials which exhibit half-metallic character. On the contrary, Ba$_2$LuTa$_{0.75}$ (Mn and Fe)$_{0.25}$O$_6$ has states at the Fermi energy in both spin directions and are thus metals. From figure 6, one can note that for Ba$_2$LuTa$_{0.75}$TM$_{0.25}$O$_6$, the core region (below $-10.0$ eV) is primarily dominated by O s, Lu p and Ba p and s state electrons for both spin channels. The valence region is essentially contributed by the Lu s and $t_{2g}$ of TM atoms. The conduction region is
mainly contributed by the d state of Ba and Ta atoms hybridisation with O s and $e_g$ of Co, Fe, Cr and Mn atoms.

The obtained total, interstitial and atom-resolved magnetic moments of Ba$_2$LuTa$_{0.75}$TM$_{0.25}$O$_6$ are shown in table 3. The total magnetic moments, 2.00 and 1.00 $\mu_B$, per unit cell for Ba$_2$LuTa$_{0.75}$(Co, Cr)$_{0.25}$O$_6$ alloys are close to an integer which agrees with the half-metallicity of these materials. The principal contribution to the total magnetic moment comes from the Co, Fe, Cr and Mn atoms and minor contributions are from the interstitial region, whereas the moments of Ba, Lu, Ta and O are small. Our results for the magnetic moment for manganese atoms agree with the experimental data of 2.6 $\mu_B$ reported in ref. [43]. The magnetic moments of the cobalt, iron and chromium atoms are in reasonable agreement with the theoretical data reported in refs [27,44]. On the other hand, this large gap in these alloys containing a localised magnetic orbital due to p–d hybridisation between the transition metal and oxygen atoms [15] is essential for the gap formation as the d–d hybridisation previously discussed [45].

Figures 7a and 7b are respectively plots of the computed real and imaginary parts of complex dielectric function as a function of photon energy in the range 0–28 eV for both pristine and doped Ba$_2$LuTaO$_6$ obtained from the electronic band structure calculated using the GGA+ $U$ approach.

It is evident in Ba$_2$LuTa$_{0.75}$Mn$_{0.25}$O$_6$ spin-up and Ba$_2$LuTa$_{0.75}$Co$_{0.25}$O$_6$ spin-down that the largest peak

![Figure 5. Total density of states (TDOS) for (a) Ba$_2$LuTa$_{0.75}$Co$_{0.25}$O$_6$, (b) Ba$_2$LuTa$_{0.75}$Cr$_{0.25}$O$_6$, (c) Ba$_2$LuTa$_{0.75}$Fe$_{0.25}$O$_6$ and (d) Ba$_2$LuTa$_{0.75}$Mn$_{0.25}$O$_6$.](image-url)
appears in the low energy region from 0 to 1 eV and then decreases sharply to attain a negative peak by increasing the energy up to 10–12 eV. For the perovskite $\text{Ba}_2\text{LuTa}_{0.75}\text{TM}_{0.25}\text{O}_6$ ($\text{TM} = \text{Co, Fe, Cr and Mn}$) alloys according to figures 7a and 7b, the static dielectric constants $\varepsilon_1(0)$ for spin-up (or spin-down) are 3.88(4.75), 3.96(3.85), 6.5(4.10) and 4.78(4.40), respectively (see table 2). The maximum values $\varepsilon_2^{\text{MAX}}(\omega)$ of $\varepsilon_2(\omega)$ are 1.55(0.62), 1.23(2.55), 0.29(2.80) and 1.95(1.08) eV for spin-up (or spin-down), respectively (see table 2). In addition, from the spectrum of the imaginary part of the dielectric function, we can see that the threshold energy which is represented by the first critical point occurs at approximately $A_1$, $A_2$, $A_3$ and $A_4$ points, respectively. These points come essentially from the transition of electrons between the three levels of the valence band and the four levels of the conduction band (see table 4). On the other hand, according to figures 7a and 7b, the static dielectric constants $\varepsilon_1(0)$ increase after TM doping. Furthermore, the relatively lower values in the energy range 0–3 eV compared to the $\text{Ba}_2\text{LuTaO}_6$ alloy, especially for the spin-down polarisation, imply that by doping with a transitional metal, the absorption feature decreases.

![Figure 6](image_url) Figure 6. Partial density of states (PDOS) for (a) $\text{Ba}_2\text{LuTa}_{0.75}\text{Co}_{0.25}\text{O}_6$, (b) $\text{Ba}_2\text{LuTa}_{0.75}\text{Fe}_{0.25}\text{O}_6$, (c) $\text{Ba}_2\text{LuTa}_{0.75}\text{Cr}_{0.25}\text{O}_6$ and (d) $\text{Ba}_2\text{LuTa}_{0.75}\text{Mn}_{0.25}\text{O}_6$ with both spin-up and spin-down channels.
Table 2. The calculated static dielectric constants $\varepsilon_1(0)$, static refractive indexes $n(0)$ and energy band gap $E_g$ (eV) for both pristine and doped Ba$_2$LuTaO$_6$.

<table>
<thead>
<tr>
<th>Material</th>
<th>$\varepsilon_1(0)$ (↑)</th>
<th>$\varepsilon_1(0)$ (↓)</th>
<th>$n(0)$ (↑)</th>
<th>$n(0)$ (↓)</th>
<th>$E_g$ (eV) (↑)</th>
<th>$E_g$ (eV) (↓)</th>
<th>$E_g$ (eV) [41]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ba$_2$LuTaO$_6$</td>
<td>2.85</td>
<td>2.85</td>
<td>1.69</td>
<td>1.69</td>
<td>3.42</td>
<td>3.42</td>
<td>2.8</td>
</tr>
<tr>
<td>Ba$<em>2$LuTa$</em>{0.75}$Co$_{0.25}$O$_6$</td>
<td>3.88</td>
<td>4.75</td>
<td>1.96</td>
<td>2.17</td>
<td>0.52</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Ba$<em>2$LuTa$</em>{0.75}$Fe$_{0.25}$O$_6$</td>
<td>3.96</td>
<td>3.85</td>
<td>1.96</td>
<td>1.96</td>
<td>–</td>
<td>1.6</td>
<td>–</td>
</tr>
<tr>
<td>Ba$<em>2$LuTa$</em>{0.75}$Cr$_{0.25}$O$_6$</td>
<td>6.50</td>
<td>4.10</td>
<td>2.54</td>
<td>2.02</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Ba$<em>2$LuTa$</em>{0.75}$Mn$_{0.25}$O$_6$</td>
<td>4.78</td>
<td>4.40</td>
<td>2.18</td>
<td>2.09</td>
<td>–</td>
<td>–</td>
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</tbody>
</table>

Table 3. Individual and net magnetic moments ($\mu_B$) of Ba$_2$LuTa$_{0.75}$TM$_{0.25}$O$_6$ alloys.

<table>
<thead>
<tr>
<th>Material</th>
<th>$m_{(TM)}$</th>
<th>$m_{Ta}$</th>
<th>$m_{Lu}$</th>
<th>$m_{Ba}$</th>
<th>$m_{o}$</th>
<th>$m_{inter}$</th>
<th>$m_{Total}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ba$<em>2$LuTa$</em>{0.75}$Co$_{0.25}$O$_6$</td>
<td>1.385</td>
<td>–0.0003</td>
<td>0.0002</td>
<td>0.0021</td>
<td>0.0027</td>
<td>0.09941</td>
<td>2.00</td>
</tr>
<tr>
<td>Ba$<em>2$LuTa$</em>{0.75}$Fe$_{0.25}$O$_6$</td>
<td>2.549</td>
<td>0.0012</td>
<td>0.0023</td>
<td>–0.0055</td>
<td>0.0004</td>
<td>0.16053</td>
<td>3.00</td>
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<tr>
<td>Ba$<em>2$LuTa$</em>{0.75}$Cr$_{0.25}$O$_6$</td>
<td>1.204</td>
<td>0.0025</td>
<td>–0.0002</td>
<td>–0.0063</td>
<td>–0.004</td>
<td>0.10345</td>
<td>1.00</td>
</tr>
<tr>
<td>Ba$<em>2$LuTa$</em>{0.75}$Mn$_{0.25}$O$_6$</td>
<td>2.384</td>
<td>–0.0003</td>
<td>–0.0054</td>
<td>–0.0005</td>
<td>–0.007</td>
<td>0.12011</td>
<td>2.12</td>
</tr>
</tbody>
</table>
The refractive index \( n(\omega) \) describes how much material is transparent or opaque. Figure 8 illustrates the refractive index \( n(\omega) \) for both pristine and doped Ba\(_2\)LuTaO\(_6\) alloy. From the refractive index plot, we remark that the material possesses high refractive index within the microwave region and decreases at higher energy in the middle ultraviolet region (4.13–6.20 eV). In addition, the static refractive indexes \( n(0) \) for spin-up (or spin-down) are 1.96(2.17), 1.98(1.96), 2.54(2.02) and 2.18(2.09), respectively (see table 2). It is clearly seen that the calculated spectra show pronounced peaks originating from the excitonic transitions at the \( E_0 \) edges. The strongest peaks in \( n(\omega) \) spectra are related mainly to the 2D exciton transition \( (E_1) \) [46]. Furthermore, after 10.00 eV within the far ultraviolet region the velocity of light is greater than the light celerity because \( n(\omega) \approx 1 \).

Figure 9 describes the energy loss of fast electrons that traverse the material under study. Accordingly, one can observe a prominent peak at photon energies 22.71, 22.87, 22.70, 22.52 and 22.49 eV, for Ba\(_2\)LuTa\(_{0.75}\)TM\(_{0.25}\)O\(_6\) (TM = Co, Cr, Mn and Fe) and Ba\(_2\)LuTaO\(_6\), respectively. The peaks shown in figure 9 are the characteristics that are linked to the plasma resonance (PR) with a frequency known as \( \omega_p \). The energy-loss spectrum is defined as the bulk plasma frequency and occurs at \( \varepsilon_1(\omega) = 0 \) and \( \varepsilon_2(\omega) < 1 \) [47]. This suggests that there is a quick reduction in the reflectance. It is to be noted that in technological applications the optical properties of the perovskite Ba\(_2\)LuTa\(_{0.75}\)TM\(_{0.25}\)O\(_6\)

![Image of graphs showing energy loss and refractive index](image-url)

**Figure 7.** The real part \( \varepsilon_1(\omega) \) and imaginary part \( \varepsilon_2(\omega) \) of dielectric constant \( \varepsilon(\omega) \) for (a) Ba\(_2\)LuTa\(_{0.75}\)Co\(_{0.25}\)O\(_6\), (b) Ba\(_2\)LuTa\(_{0.75}\)Fe\(_{0.25}\)O\(_6\), (c) Ba\(_2\)LuTa\(_{0.75}\)Cr\(_{0.25}\)O\(_6\) and (d) Ba\(_2\)LuTa\(_{0.75}\)Mn\(_{0.25}\)O\(_6\).
Figure 7. Continued.

Table 4. Position of the principal peaks of the imaginary part of the dielectric function for Ba$_2$LuTa$_{0.75}$TM$_{0.25}$O$_6$ compounds.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Energy (eV)</th>
<th>Transition</th>
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<tbody>
<tr>
<td>Ba$<em>2$LuTa$</em>{0.75}$Co$_{0.25}$O$_6$</td>
<td>GGA + $U$</td>
<td>0.64</td>
</tr>
<tr>
<td>Transitions</td>
<td>Co-$t_{2g}$ → Co-$e_g$</td>
<td>Lu-$s$ → Co-$e_g$</td>
</tr>
<tr>
<td></td>
<td>GGA-PBE</td>
<td>0.95</td>
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<tr>
<td>Transitions</td>
<td>Cr-$t_{2g}$ → Co-$e_g$</td>
<td>Lu-$s$ → Cr-$e_g$</td>
</tr>
<tr>
<td>Ba$<em>2$LuTa$</em>{0.75}$Fe$_{0.25}$O$_6$</td>
<td>GGA-PBE</td>
<td>0.57</td>
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<tr>
<td>Transitions</td>
<td>Fe-$t_{2g}$ → F-$e_g$</td>
<td>Lu-$s$ → Fe-$e_g$</td>
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<td></td>
<td>GGA-PBE</td>
<td>0.30</td>
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<tr>
<td>Transitions</td>
<td>Mn-$t_{2g}$ → F-$e_g$</td>
<td>Lu-$s$ → Mn-$e_g$</td>
</tr>
</tbody>
</table>
Figure 8. Calculated refractive index $n(\omega)$ for both pristine and doped Ba$_2$LuTaO$_6$.

Figure 9. Energy loss function $L(\omega)$ for both pristine and doped Ba$_2$LuTaO$_6$. 
alloys are the most suitable for exploring appropriate conditions in optoelectronics domain.

4. Conclusion

In summary, we have performed first-principles calculations of the Ba$_2$LuTa$_{0.75}$(Co, Cr)$_{0.25}$O$_6$ alloys to explore their structural, electronic, half-metallic and optical properties. Our results showed that the Ba$_2$LuTa$_{0.75}$(Co, Fe and Cr)$_{0.25}$O$_6$ alloys are indirect half-metallic materials with a band gap of 0.52(↑) and 1.6(↓) eV, respectively, while Ba$_2$LuTa$_{0.75}$Mn$_{0.25}$O$_6$ exhibits a metallic behaviour suggesting that the Ba$_2$LuTa$_{0.75}$(Co and Cr)$_{0.25}$O$_6$ are good candidate materials for future spintronic applications. Dielectric function, refractive index and loss of energy are calculated and discussed.

References

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