| 1  | The effect of hydrostatic pressure on the electronicproperties of  |
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| 2  | TIBr and TICI radiation detectors  |
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| 8  |  |
| 9  | Abstract   |
| 10   |  |
| 11<br>12<br>13<br>14<br>15<br>16<br>17<br>18 | We present first principles calculations of the electronic properties of TlBr and TlCl binary semiconductor compounds. The dependences on hydrostatic pressure of these properties (band structure, density of states, electronic charge density) are successfully calculated using self-consistent scalar relativistic full potential linear augmented plane wave method (FP-LAPW) within the generalized gradient approximation (GGA). The GGA corrections yield only minor improvement, whereas Engel-Vosko approximation gives a significant improvement to the band gap. The results are compared with previous calculations and with experimental measurements, we found good agreement with our calculations. |
| 19<br>20                                     |  |
| 21   | Keywords: band structure, density of states, electronic charge density, radiation detectors.   |
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# 36 **1-INTRODUCTION**

Thallium halides (TICl and TIBr) are technologically very important materials having many applications as radiation detectors and as new optical fibre crystals. Thallium chloride and thallium bromide both, crystallize in the cubic CsCl structure. This structure, with a coordination number of eight, represents the most stable dense configuration for ionic crystals [1–3].

In the past two decades there has been much interest in the pressure dependence of the optical properties semiconductors [4-9]. While the fundamental understanding of this problem is in itself of great importance, with the recent development of strained superlattices it has become more relevant.

High-pressure studies are a very efficient tool inunderstanding the electronic and optical
properties of semiconductors [10], but they have been scarcely used in the investigation ofTlBr
and TlCl, compared to other II–VI semiconductors.

The study of materials at high pressures has a great activitybecause of the developments of the diamond-anvil technique and the extension of the range for optical and X-ray measurements under static pressures [11,12].

The main motivation of this work is to study the change in the optical properties under pressure of two technologically important semiconductors TIBr and TICLA modification of the crystal lattice which does not change its symmetry properties can be obtained by applying hydrostatic pressure to the crystal. A pressure changes produces shifts of the electronic states and, hence a change in the optical properties of the crystal. Therefore pressure provides a convenient technique for modifying optical constants by a controlled amount.

58 Most of the heavy-metal halides crystallize into anisotropic or layered structures. The 59 simple lattice structure would reduce the complexity of electronic structure usually encountered 60 in anisotropic materials and allow us a simple analysis of the optical spectra. Optical properties 61 of TIC1 and T1Br have been studied by many workers in the absorption edge [13] and in the 62 VUV region [14].A remarkable property of thallium halide crystals is their high dielectric 63 permittivity. The static values are 30 and 32 for the cubic T1Br and T1Cl [15-16].

64 In this study, we have investigated the optical properties by means of first-principles 65 density-functional total-energy calculation using the all-electron full potential linear augmented 66 plane-wave method (FPLAPW) [17].

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#### 81 **2- CALCULATIONS**

The calculation of the pressure of optical properties is a long standing problem in semiconductor physics. Although detailed calculations of the pressure dependence of optical properties with varying degree of sophistication like empirical pseudopotential [18], selfconsistent first principle pseudopotential [19,20] and quasiparticle [21,22] have successfully estimated some coefficients, the results are not entirely satisfactory.

A modification of the crystal lattice which does not change its symmetry properties can be
 obtained by applying hydrostatic pressure to the crystal. A pressure changes the lattice
 parameters and, hence produces shifts of the electronic states in the crystal.

91 Scalar relativistic calculations have been performed using the wien2k code [23,24]. For 92 the exchange correlation potential, we have used the local density approximation (LDA) with a 93 parameterization of Ceperly-Adler data [25]. The new Full Potential Augmented Plane Wave 94 method of the density functional theory is applied [26,27]. Several improvements to solve the 95 energy dependence of the basis set were tried but the first really successful one was the 96 linearization scheme introduced by Andersen[28] leading to the linearized augmented plane 97 wave (LAPW) method. In LAPW, the energy dependence of each radial wave function inside the 98 atomic sphere is linearized by taking a linear combination of a solution u at a fixed linearization 99 energy and its energy derivative  $\dot{u}$  computed at the same energy.

$$100 \qquad \Phi_{K}(\mathbf{r}) = \begin{cases} \sum_{L} \left[ a_{L}^{\alpha K} u_{1}^{\alpha}(r') + b_{L}^{\alpha K} \dot{u}_{1}^{\alpha}(r') \right] Y_{L}(\hat{r}') & r' \langle R_{\alpha} \\ \Omega^{-1/2} \exp(i(k+K).r) & r \in I \end{cases}$$
(1)

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Where r'=r-r<sub> $\alpha$ </sub> is the position inside sphere  $\alpha$  with polar coordinates r' and r, **k** is a wave vector in 102 the irreducible Brillouin zone, **K** is a reciprocal lattice vector and  $u_1^{\alpha}$  is the numerical solution to 103 the radial Schrodinger equation at the energy  $\varepsilon$ . The coefficients  $a_{L}^{\alpha K}$  are chosen such that the 104 atomic functions for all L components match (in value) the PW with K at the Muffin tin sphere 105 boundary. The KS orbitals are expressed as a linear combinations of APWs  $\Phi_{\kappa}(\mathbf{r})$ . In 1991 106 Singh [29] introduced the concept of local orbitals (LOs) which allow an efficient treatment of 107 108 the semi-core states. An LO is constructed by the LAPW radial functions u and  $\dot{u}$  at one energy 109  $\varepsilon_1$  in the valence band region and a third radial function at  $\varepsilon_2$ .

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$$\Phi_{\rm LO}(\mathbf{r}) = \begin{cases} \left[ a_{\rm L}^{\alpha,\rm LO} u_{\rm 1l}^{\alpha}(\mathbf{r}') + b_{\rm L}^{\alpha,\rm LO} \dot{u}_{\rm 1l}^{\varepsilon}(\mathbf{r}') + c_{\rm L}^{\alpha,\rm LO} u_{\rm 2l}^{\alpha}(\mathbf{r}') \right] Y_{\rm L}(\hat{\mathbf{r}}') & \mathbf{r}' \langle \mathbf{R}_{\alpha} \\ 0 & \mathbf{r} \in \mathbf{I} \end{cases}$$
(2)

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Recently, an alternative approach was proposed by Sjöstedt et al [30], namely the APLW+ lo (local orbital) method. Here the augmentation is similar to the original APW scheme but each radial wavefunction is computed at a fixed linearization energy to avoid the non-linear eigenvalue problem. The missing variational freedom of the radial wavefunctions can be recovered by adding another type of local orbitals (termed in lower case to distinguish them from LO) containing u and ù term:

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$$\Phi_{lo}(\mathbf{r}) = \begin{cases} \left[ a_{L}^{\alpha,lo} u_{l}^{\alpha}(\mathbf{r}') + b_{L}^{\alpha,lo} \dot{u}_{l}^{\alpha}(\mathbf{r}') \right] Y_{L}(\mathbf{r}') & r' \langle R_{\alpha} \\ 0 & r \in I \end{cases}$$
(3)

122 It was demonstrated that this new scheme converges faster than LAPW. The APW +lo scheme123 has been implemented in the wien2k code version [31].

124 However, in the calculations reported here, we chose the muffin tin radii for Tl, Br and Cl 125 to be 2.5 a.u.. The expansion of the spherical region is developed up to  $l_{max}=10$  for both 126 compounds, while in the interstitial region we have used 372 plane waves for TlBr and 331 for

127 TICl. Furthermore, we have used the energy cut-off of  $R_{MT}.K_{\mu\alpha\xi}=8$  and the maximal 128 reciprocal vector equal to 10 for both compounds.

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## 131 **3. RESULTS**

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The structural optimization of the cubic phase was performed by calculating the 133 totalenergy as function of the volume. The minimization of the total energy versus volume 134 135 requires that each of the self-consistent calculations is converged, so the iteration process was 136 repeated until the calculated total energy of the crystal converged to less than 1 mRyd.A total of 137 seven iterations were necessary to achieve self-consistency for TlBr and nine iterations in the 138 case of TICI. The equilibrium lattice constants and bulk modulus are calculated by fitting the 139 total energy versus volume according to Murnaghan's equation of state [33]. The variation of 140 total energy as a function of volumeis shown in figures 1a and 1b for TlBr and TlCl 141 respectively.

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Our results are shown along with other theoretical values in Tables 1 and 2. It is found that for the generalized gradient approximation (GGA92) and (GGA96), the energy gap is underestimated relative to the experimental value due to the well known artifact of the local density approximation calculations, while the Engel-Vosko scheme gives quite a nice band gap compared to the experimental one.

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## 150 3.1 <u>Electronic band structures</u>

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The electronic band structures of cubic TlBr and TlCl along symmetry lines are shown in figures 2a, 2b at normal pressure and 3a, 3b under hydrostatic pressure. The calculated band energy gap at high symmetry points is given in table 2; the band gap is found to be direct and equal to 1.87 eV and 2.08 eV for TlBr and TlCl respectively, which is in close agreement with other theoretical calculations as shown in table 2.

157 It is clear from these figures that the energy levels are shifted upon applied pressure for both Tl

158 Br and TlCl; under pressure, the energy levels for the valence bands decrease while the ones of

159 the conduction bands increase, the main band gaps are also increased under pressure, hence The

160 valence bandwidth increases with the increase of pressure, while the conduction bandwidth

161 decreases with the increase of pressure.

162 The band structure is qualitatively similar to that of ambient pressure. However, the conduction 163 minimum at C shifts upwards, while the X-point conduction-band minimum moves down relative to the valence-band maximum. The energy of the lowest conduction band at the L point is almost independent of pressure.

166 We applied a pressure up to 8.69 GPa for TlBr and 10.33 GPa for TlCl, because this structure

167 transforms to another phase when pressure exceeds those values. The variation is not constant and

depends on the k-point and energy. Both materials under study remain a direct band-gap at 8.69

169 GPa for TlBr and 10.33 GPa for TlCl.

170 It is interesting to compare our calculated gaps with experimental data (see table 2). Since 171 quasi-particle excitations are not taken into account in density functional theory (DFT), the 172 energy gap calculated from DFT, often called the Kohn-Sham gap, tends to be smaller than the 173 experimental one. In some cases, even the wrong ground state is predicted, as, e.g., in Ge, where 174 the energy gap is around 0.7 eV, whereas the LDA Kohn-Sham gap is slightly negative at 175 ambient pressure [26]. The GGA corrections yield only minor improvement. Quasiparticle 176 calculations essentially overcome the underestimate of the band gap as obtained using the LDA, 177 The GW [27] calculations for GaN for instance yield band structures in much better agreement with experiment; they are, however, time consuming and do not, as yet, produce selfconsistent 178 179 total-energy values. However, in our case, the use the Engel-Vosko improves significantly the 180 band gap which becomes closer to the experimental one.

Figure 2a indicates that TlBr with cubic structure has a direct band gap between the top of the valence band and the bottom of the conduction band at the X. The lowest band is the Tl 6sband. At X there is significant mixing between the nominal Tl s and the  $X_6^+$  which is the valence band edge. A maximum pressure of 8.69 GPa was used.

185 In the case of TlCl (figure 3a), the overall results are similar to TlBr; table 2 summarizes the key information for TICI, discrepancies between calculated and experimental band gap, 186 which can be attributed as stated earlier to the exchange GGA potentials which do not take into 187 188 account the excitations, whereas the Engel-vosko correction significantly improves the gap 189 which is 2.72 eV and 2.96 eV for TlBr and TlCl respectively different from the experimental 190 ones. Note that in the case of TlCl, the Cl s and p bands make the convergence of the calculation 191 a bit longer. The calculated band gaps at p=8.69 GPa and p=10.33 GPa for TlBr and TlCl are 192 given in table 3.

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**Table 1:**Static equilibrium constant a (Å) for TlBr and TlCl. Comparison of present results
 with previous calculations.

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| Compounds               | TlBr                       |                    |                   | TICI                       |                    |                   |
|-------------------------|----------------------------|--------------------|-------------------|----------------------------|--------------------|-------------------|
|                         | Present<br>work<br>(GGA96) | Other calculations | Exp.              | Present<br>work<br>(GGA96) | Other calculations | Exp.              |
| Lattice parameter a (Å) | 4.0                        | 3.96 <sup>c</sup>  | 3.98 <sup>a</sup> | 3.84                       | 3.84 <sup>c</sup>  | 3.83 <sup>b</sup> |

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<sup>a</sup>reference [28]

<sup>b</sup>reference [29]

202 <sup>c</sup>reference [30]

### Table 2. Band energies (eV) for TlBr and TlCl

| TlBr            | Present work | <b>Present work</b> | <b>Present work</b>    | Other calculations         | Experiment        |
|-----------------|--------------|---------------------|------------------------|----------------------------|-------------------|
| Energy gap (eV) | 1.87 (GGA96) | 1.74 (GGA92)        | 2.72 (Engel-<br>Vosko) | 2.38 eV (OPW) <sup>a</sup> | 2.68 <sup>b</sup> |

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| TICI            | Present work | Present work | <b>Present work</b>    | Other calculations                 | Experiment        |
|-----------------|--------------|--------------|------------------------|------------------------------------|-------------------|
| Energy gap (eV) | 2.08 (GGA96) | 1.94 (GGA92) | 2.96 (Engel-<br>Vosko) | $2.04 \text{ eV} (\text{OPW})^{a}$ | 3.22 <sup>b</sup> |
|                 |              |              | ( OBRO)                |                                    |                   |

| 207 |   |
|-----|---|
| 200 | а |

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| 208 | <sup>a</sup> Reference [30] |  |
|-----|-----------------------------|--|
| 209 | <sup>b</sup> Reference [31] |  |
| 210 |                             |  |
| 211 |                             |  |
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| 213 |                             |  |
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| 215 | 3.2 Total charge density    |  |
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To visualize the nature of the bond character and to explain the charge transfer and the bonding 217 properties of cubic TlBr and TlCl, we calculate the total charge density. 218

The electronic charge density is obtained for each band n by summing over the k-states in the 219 220 band.

(6)

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$$\rho_n(r) = \sum \left| \Psi_{nk}(r) \right|^2$$

222 and the total charge density is obtained by summing over the occupied band.

223 
$$\rho(r)$$

 $=\sum \rho_n(r)$ (7)224 The total valence charge densities for the two binary compounds, TlBr and TlCl, are displayed along the TI-Br-Cl bonds in figures 3a and 3b. 225

226 Figures4a and 4b show the charge density distribution in the (110) plane for TlBr and 227 TICI respectively at normal pressure and at 8.69 GPa for TIBr and 10.33 GPa for TICI. The 228 calculated electron charge distributions indicate that there is a strong ionic character for both 229 compounds as can be seen along the Tl-Br-Cl bonds. The charge densities around the atoms have 230 asymmetric forms which are similar to those given in previous reports using the ab initio pseudo-231 potential method [32]. The charge transfer gives rise to the ionic character in TIBr and TICI semiconductor compounds. The driving force behind the displacement of the bonding charge is 232 233 the greater ability of Tl to attract electrons towards it due to the difference in the 234 electronegativity of Tl and Br. However as pressure is applied we note a charge transfer toward 235 the interstitial region, and also a decrease in the charge density, more noticeable in the case of

TIBr, this is attributed to the difference in the core size of these compounds. The charge distribution which was concentrated at the atomic sites at normal pressure becomes more delocalized throughout the unit cell. This difference has important physical consequences, the substitution of the interstitial sites of TIBr and TICl with host atoms can affect the band structure topology and gives rise to a semiconductor with new physical properties.

The total DOS curves displayed on figures 5a and 5b give an idea about the dominant orbital character of the groups of bands in the indicated regions of energy for TlBr and TlCl, respectively.

244 The cubic binary compounds TIBr and TICl have valence band densities of states qualitatively

similar to the band structures. The energy zero is the top of the valence band,  $E_v$ , or valence-band maximum (VBM). Structures of the density of states are labeled with the same notation as the

band structure and the corresponding points in the Brillouin zone follow from inspection of the

band structure. The minimum of the density of states occurs at  $\Gamma$  at -5.3 eV for TlBr and -5.2 eV for TlCl. The lower states from -5.3 to -2.7 eV and from -5.2 to -2.71 eV for TlBr and TlCl,

eV for TlCl. The lower states from -5.3 to -2.7 eV and from -5.2 to -2.71 eV for TlBr and TlCl, respectively have primarily s character and are localized on the anion. The second state of the second valence band is cation s, it changes rapidly to anion p-like at the top of the valance band

in the case of TlCl. However, as pressure is applied, the intensity of the peaks in the DOS figure
 decreases and also both valence and conduction band peaks are shifted as sated above in the band
 structure analysis.

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Table 3: The calculated band energies for TlBr and TlCl at different
pressures (Present work GGA96).

|               | TlBr       |               | TlCl       |
|---------------|------------|---------------|------------|
| Pressure(GPa) | Energy gap | Pressure(GPa) | Energy gap |
| 0             | 1.87       | 0             | 2.08       |
| 8.69          | 0.76       | 10.33         | 0.87       |

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261

# 262 Conclusion

263

264 The effect of hydrostatic pressure on the electronic properties of cubic TlBr and TlCl have been investigated using the wien2k package, full-potential linearized augmented plane wave (FP-265 LAPW) approach within the density functional theory (DFT) in the local spin density 266 267 approximation (LSDA) including the generalized gradient approximation (GGA) was used. The 268 use of GGA for the exchange-correlation potential permitted us to obtain good structural 269 parameters but an underestimated fundamental band gap, whereas the Engel-vosko correction 270 significantly improves the gap. The charge densities have been presented and provide additional 271 evidence of the similarity of the bonds in TlBr and TlCl. As a result of the ionic character of these two binary semiconductor compounds which share many similar properties. We noticed 272 273 that at much lower pressures, the character of the fundamental gap is affected by changes in band 274 dispersion of the topmost part of the valence band in both TlBr and TlCl.

- 275 However, the charge distribution which was concentrated at the atomic sites at normal pressure
- 276 becomes more delocalized throughout the unit cell as pressure is applied, this has important 277 physical consequences, substitution of the interstitial sites with host atoms will give rise to a
- 278 semiconductor with different physical properties.
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- 284 285

#### 286 **Figure captions**

- **Figure 1a:** Energy (eV) versus Volume ( $Å^3$ ) for TlBr 287
- **Figure 1b**: Energy (eV) versus Volume  $(Å^3)$  for TlCl 288
- **Figure 2a:**Energy (eV) versus Wave vector for TIBr at normal pressure (GGA-08) 289
- 290 Figure 2b:Energy (eV) versus Wave vector for TlCl at normal pressure (GGA-08)
- 291 Figure 3a: Energy (eV) versus Wave vector for TlBr at pressure p=8.69 GPa, (GGA-08)
- 292 **Figure 3b**: Energy (eV) versus Wave vector for TlCl at pressure p=10.33 GPa, (GGA-08)
- 293 Figure 4a: Electron density (arb. Units) versus Position (a.u.) for TlBr at normal pressure and at
- 294 p= 8.69 GPa (GGA-08)
- 295 Figure 4b: Electron density (arb. Units) versus Position (a.u.) for TlCl at normal pressure and at 296 p = 10.33 GPa (GGA-08)
- Figure 5a: Density of states for TlBr at normal pressure and at p= 8.69 GPa (GGA-08) 297
- 298 Figure 5b: Density of states for TlCl at normal pressure and at p= 8.69 GPa (GGA-08)
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