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***Research paper***

# Mechanical and thermal properties versus effective cubic lattice constant in $Cu_2$-II-IV-$VI_4$ quaternary compounds

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**Abstract**

The present work aims to study the dependence of the bulk modulus B and the Debye temperature $\theta_D$ with the effective cubic lattice constant $a_{eff}$ of some $Cu_2$-II-IV-$VI_4$ compounds. We are also studied the correlation between the bulk modulus B, the Debye temperature $\theta_D$, the microhardness H and the melting point $T_m$.
The fits of the data of the bulk modulus B and the Debye temperature $\theta_D$ versus the effective cubic lattice constant $a_{eff}$ show that B of $Cu_2$-II-IV-$VI_4$ semiconducting materials decreases almost linearly with increase of the effective cubic lattice constant $a_{eff}$, while that of Debye Temperature $\theta_D$ decreases exponentially with a rising of the effective cubic lattice constant $a_{eff}$. The coefficients of the correlation were found at around -0.78 for the bulk modulus B, and at around -0.94 for the Debye temperature, respectively.
For the bulk modulus B, the best fit was obtained using the following expression: $B = - 596.52\ a_{eff} + 393.4$, where B is expressed in GPa, and $a_{eff}$ in nm, while that of $\theta_D$ is: $\theta_D = 165.46 + 3.8 \exp(-57.2\ a_{eff})$, respectively. The average error on the estimation of B was found at around 10%, while that on the estimation of $\theta_D$ is only around 4.5%, respectively. Our expressions perhaps used with high accurate to predict the bulk modulus B and the Debye temperature $\theta_D$ of other quaternary $Cu_2$-II-IV-$VI_4$ semiconducting materials.

***Keywords***: *$Cu_2$-II-IV-$VI_4$ Semiconductors; Least-Squares Fit; Thermal Properties; Effective Cubic Lattice Constant; Microhardness*

## 1. Introduction

Functional materials play an important role in developing new technologies due to their interesting physical properties [1–12]. Several works [13–20] investigated the correlation between the different properties of functional semiconducting materials. Daoud [13] has established simplified expressions for calculating Debye temperature and melting point of II-VI and III-V compounds; while in other work [14], He investigated the correlation between Debye temperature and lattice thermal conductivity in II-VI and III-V semiconductors.
Because of their applications in the fabrication of low cost solar cells and their large magneto-optical effects which are observed when II elements are paramagnetic atoms, $I_2$-II-IV-$VI_4$ (II = Zn, Cd, Hg, Mn, Fe or Co, IV = Si, Ge, Sn or Pb and VI = S, Se or Te) quaternary semiconducting materials, Quintero et al. [16] used X-ray powder diffraction measurements, at 300 K, and differential thermal analysis (DTA) to investigate the thermal properties of several polycrystalline samples of $Cu_2$-II-IV-S4(Se4) magnetic materials.
Adachi [17] studied the correlation between several physical properties of tetragonal and orthorhombic $Cu_2$-II-IV-$VI_4$ compounds and their molecular weight; while very recently, Daoud and co-authors [18] investigated the correlation between the melting point $T_m$ and the microhardness H of tetragonal and orthorhombic $Cu_2$-II-IV-$VI_4$ (II = Zn, Cd, Hg; IV = Si, Ge, Sn) compounds. They also use their model to predict the microhardness H of $Cu_2ZnSnS_4$ (CZTS) compound.
The physics of the photovoltaic effect including the spectral irradiance of solar radiation and the influence of the Earth's atmosphere on it, and several other interesting physical properties of copper zinc tin sulfide-based thin-film solar cells were presented by Ito [19]. Additionally, He explored the electronic and optical properties of the kesterite and stannite phases of $Cu_2ZnSnS_4$ and $Cu_2ZnSnSe_4$ (CZTSe) by means of first-principles modeling.
Chalapathy et al. [21] elaborate $Cu_2ZnSnS_4$ thin films by sulfurization of Cu/ZnSn/Cu precursorin sulfur atmosphere. The CZTS films obtained exhibited the Kesterite phase; and under standard AM 1.5 conditions, they found that the solar cell fabricated with the CZTS material showed a conversion efficiency of ~ 4.59% for 0.44 $cm^2$.
In the present work, we studied firstly the correlation between the bulk modulus B, the Debye temperature $\theta_D$ and the effective cubic lattice constant $a_{eff}$ of tetragonal and orthorhombic $Cu_2$-II-IV-$VI_4$ (II = Zn, Cd, Hg; IV = Si, Ge, Sn) compounds, then the correlation between the bulk modulus B and the melting point $T_m$; and the Debye temperature $\theta_D$ and the microhardness H of these materials.

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## 2. Theory, results and discussion

At normal temperature and pressure, most of the $Cu_2$–II–IV–$VI_4$ semiconducting compounds crystallize in the tetragonal or orthorhombic structures [17], [19]. The unit cell geometry of tetragonal phase was assigned as: $a = b \neq c$ (lattice constants), and $\alpha = \beta = \gamma = 90°$ (lattice angles), while in orthorhombic structure, the unit cell geometry was assigned as: $a \neq b \neq c$, and $\alpha = \beta = \gamma = 90°$ [15]. In the tetragonal phase, the effective cubic lattice constant $a_{eff}$ is calculated, using the lattice parameters a and c as follow: $a_{eff} = (a^2c/2)^{1/3}$ [17].
We compile in Table 1 the effective cubic lattice constant $a_{eff}$ [17], the melting points $T_m$[17], the microhardness H [17], the bulk modulus B [17], [22 - 24], and the Debye temperature [16], [17], [22], [23] reported for a number of $Cu_2$-II-IV-$VI_4$ compounds. It must be noted that the data of the bulk modulus B taken from the Ref.[24] are theoretical, and they are approximately reproduced from the histogram of the figure 9 reported in the work of Hasan et al. [24]

**Table 1:**Effective Cubic Lattice Constant $a_{eff}$, Melting Point $T_m$, Bulk Modulus B, Debye Temperature $\theta_D$, and Microhardness H of Some $Cu_2$-II-IV-$VI_4$ Semiconducting Compounds[17],[a] Ref [22],[b] Ref [23], [c] Ref [16], [d] Ref [24], Values with * are Theoretical

| Materials | Structure-type | $a_{eff}$(nm) | $T_m$(K) | $B_m$(GPa) | H (GPa) | $\theta_D$(K) |
|---|---|---|---|---|---|---|
| $Cu_2ZnSiS_4$ | Orthorhombic | 0.5265 | 1396 | 81 [a] * | 3.4 | 490 [a] * |
| $Cu_2ZnSiSe_4$ | Orthorhombic | 0.5539 | 1246 | 61 [b]* | 2.8 | 282 [b] * |
| $Cu_2ZnGeS_4$ | Tetragonal | 0.5313 | 1377 | 72[d]* | 3.4 | - |
| $Cu_2ZnSnS_4$ | Tetragonal | 0.5428 | 1377 | 86 | - | 302 |
| $Cu_2ZnSnSe_4$ | Tetragonal | 0.5682 | 1259 | 70 | - | 195[c] |
| $Cu_2CdSiS_4$ | Orthorhombic | 0.5364 | 1289 | 64 [d]* | 2.5 | - |
| $Cu_2CdGeS_4$ | Orthorhombic | 0.5419 | 1288 | 70 [d]* | - | 267 [c] |
| $Cu_2CdGeSe_4$ | Tetragonal | 0.5674 | 1107 | 56 [d]* | 1.9 | 198 [c] |
| $Cu_2CdSnS_4$ | Tetragonal | 0.5530 | 1190 | 62 [d]* | 2.2 | - |
| $Cu_2CdSnSe_4$ | Tetragonal | 0.5786 | 1054 | 34 [d]* | 1.5 | 182 [c] |
| $Cu_2HgSnSe_4$ | Tetragonal | 0.5678 | 985 | 55 [d]* | 1.4 | 166 [c] |
| $Cu_2HgGeSe_4$ | Tetragonal | 0.5787 | 1027 | 51 [d]* | 1.5 | - |

We examine the correlation between the bulk modulus B and the effective cubic lattice constant $a_{eff}$ of different $Cu_2$-II-IV-$VI_4$ compounds, so the data of B and $a_{eff}$ reported in Table 1are traced in Figure 1. We can observe that B decreases with the increase of $a_{eff}$. The linear fit was given as follow: $B = -596.52a_{eff} + 393.4$, where B is expressed in GPa, and $a_{eff}$ in nm. The significance of the regression is given as the probability p of the null hypothesis $p < 2.81 \times 10^{-3}$, while the coefficient of the correlation was found at around -0.78. In Table 2, we report the calculated bulk modulus B of different $Cu_2$-II-IV-$VI_4$ semiconducting compounds using our model ($B = -596.52a_{eff} + 393.4$). We also calculated the error on B, the average error on the estimation of B was found at around 10%.

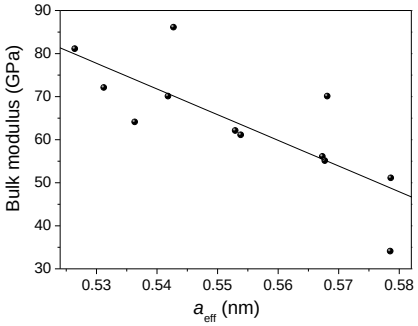



**Fig. 1:** Bulk Modulus B Versus the Effective Cubic Lattice Constant $a_{eff}$ for Some $Cu_2$-II-IV-$VI_4$ Compounds.

Several thermal properties of different materials with different crystallographic structures have been successfully determined from the cohesive energy and elastic constants [25-30]. The bulk modulus B and the melting point $T_m$ data of $Cu_2$-II-IV-$VI_4$ compounds listed in Table 1are plotted in Figure 2. We can observe that B increases with the increase of the melting point $T_m$. The linear fit was given as follows: $B = 0.084\ T_m - 38.12$, where B is expressed in GPa, and $T_m$ in K. The significance of the regression is given as the probability p of the null hypothesis $p < 3.58 \times 10^{-4}$, and a squared correlation coefficient $R^2 = 0.86$.

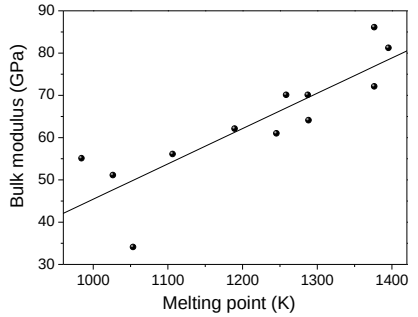



**Fig. 2:** Bulk Modulus B versus Melting Point $T_m$ for Some $Cu_2$-II-IV-$VI_4$ Semiconducting Compounds.

In Table 2, we report the calculated bulk modulus B of $Cu_2$-II-IV-$VI_4$ compounds using $B = 0.084T_m - 38.12$ model, along the results obtained from our first model ($B = -596.52a_{eff} + 393.4$). We also calculated the errors on B, the average errors on the estimation of B were found at around 9.75% from our second model ($B = 0.084T_m - 38.12$) and 10% from our first model ($B = -596.52a_{eff} + 393.4$), respectively. Our expressions related B, $a_{eff}$ and $T_m$ can be used to predict the bulk modulus B of other $Cu_2$-II-IV-$VI_4$ compounds.

The Debye temperature $\theta_D$ and the effective cubic lattice constant $a_{eff}$ data of some $Cu_2$-II-IV-$VI_4$ reported in Table 1 are plotted in Figure 3. We can observe clearly that $\theta_D$ decreases not linearly with the increase of the effective cubic lattice constant $a_{eff}$. The best exponential fit with an expression having three adjustable parameters of $\theta_D$ (expressed in K) versus $a_{eff}$ (expressed in nm) was given as follows: $\theta_D = 165.46 + 3.8 \exp(-57.2\ a_{eff})$. The significance of the regression is given with a coefficient of the correlation of around -0.94.

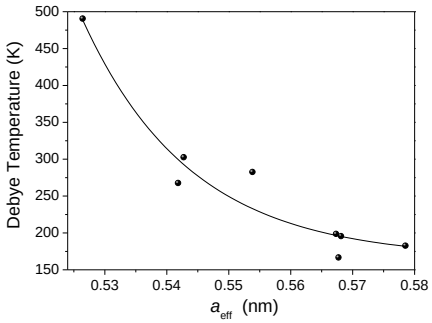



**Fig. 3:** Debye Temperature $\theta_D$ Versus the Effective Cubic Lattice Constant $a_{eff}$ for Some $Cu_2$-II-IV-$VI_4$ Compounds.

We also calculated the error on the Debye Temperature $\theta_D$, the average error on $\theta_D$ was found at around 4.5%. Our expression related $\theta_D$ and $a_{eff}$ can be used to predict the Debye Temperature $\theta_D$ of other $Cu_2$-II-IV-$VI_4$ semiconducting compounds.
The Debye Temperature $\theta_D$ and the microhardness H data listed in Table 1are plotted in Figure 4. We observe that Debye Temperature $\theta_D$ rises also not linearly with increase of the microhardness H. The polynomial fit was given as follows: $\theta_D = - 416.5 + 879.8\ H - 434.4\ H^2 + 74.7\ H^3$, where $\theta_D$ is expressed in K, and H in GPa. The significance of the regression is given with a coefficient of the correlation of around 0.999, and the probability p of the null hypothesis $p < 0.0244$. Our expression related $\theta_D$ and H was used to predict the Debye Temperature $\theta_D$ of $Cu_2ZnGeS_4$, $Cu_2CdSiS_4$ and $Cu_2CdSnS_4$ compounds. The results were found: 489 K for $Cu_2ZnGeS_4$, 235 K for $Cu_2CdSiS_4$, and 212 K for $Cu_2CdSnS_4$, respectively. To the best of our knowledge, there are no data available in the literature on $\theta_D$ for $Cu_2ZnGeS_4$, $Cu_2CdSiS_4$, and $Cu_2CdSnS_4$ materials.

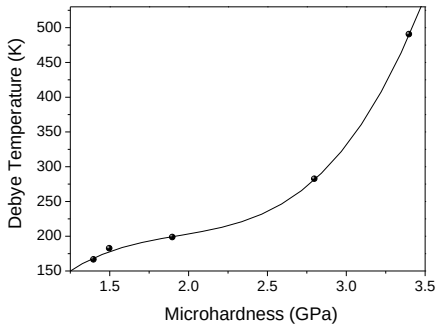



**Fig. 4:** Debye Temperature $\theta_D$ versus the Microhardness H for Some $Cu_2$-II-IV-$VI_4$ Semiconducting Compounds.

**Table 2:** Calculated Bulk Modulus B (GPa) and Debye Temperature $\theta_D$(K) and the Errors on B and on $\theta_D$ for Some $Cu_2$-II-IV-$VI_4$ Semiconductors

| Material | $B_{Calc}$* | Error (%)*on B | $B_{Calc}$** | Error (%)on B** | $\theta_{DCalc}$ *** | Error (%) on $\theta_D$*** | $\theta_{DCalc}$**** | Error (%) on $\theta_D$**** |
|---|---|---|---|---|---|---|---|---|
| $Cu_2ZnSiS_4$ | 79 | 2.06 | 79 | 2.29 | 492 | 0.38 | 489 | 0.17 |
| $Cu_2ZnSiSe_4$ | 63 | 3.26 | 67 | 9.09 | 234 | 17.14 | 281 | 0.33 |
| $Cu_2ZnGeS_4$ | 76 | 6.21 | 78 | 7.71 | 414 | - | 489 | - |
| $Cu_2ZnSnS_4$ | 70 | 19.06 | 78 | 9.83 | 294 | 2.63 | - | - |
| $Cu_2ZnSnSe_4$ | 54 | 22.20 | 68 | 3.38 | 196 | 0.30 | - | - |
| $Cu_2CdSiS_4$ | 73 | 14.73 | 70 | 9.62 | 351 | - | 235 | - |
| $Cu_2CdGeS_4$ | 70 | 0.21 | 70 | 0.10 | 301 | 12.67 | - | - |
| $Cu_2CdGeSe_4$ | 55 | 1.90 | 55 | 2.02 | 197 | 0.51 | 199 | 0.66 |
| $Cu_2CdSnS_4$ | 64 | 2.46 | 62 | 0.26 | 237 | - | 212 | - |
| $Cu_2CdSnSe_4$ | 48 | 41.92 | 50 | 48.28 | 182 | 0.05 | 178 | 2.25 |
| $Cu_2HgSnSe_4$ | 55 | 0.55 | 45 | 18.87 | 196 | 18.24 | 169 | 1.67 |
| $Cu_2HgGeSe_4$ | 48 | 5.50 | 48 | 5.59 | 182 | - | 178 | 0.17 |

* Using $B = - 596.52 a_{eff} + 393.4$, ** Using $B = 0.084 T_m - 38.12$, *** Using $\theta_D = 165.46 + 3.8 \exp(-57.2\ a_{eff})$, **** Using $\theta_D = - 416.5 + 879.8\ H - 434.4\ H^2 + 74.7\ H^3$

## 3. Conclusion

Using the data reported in the literature, we investigate the dependence between the bulk modulus B, the Debye temperature $\theta_D$ and the effective cubic lattice constant $a_{eff}$ of $Cu_2$-II-IV-$VI_4$ (II = Zn, Cd, Hg; IV = Si, Ge, Sn) compounds. We found that the bulk modulus B decreases almost linearly with the increase of the effective cubic lattice constant $a_{eff}$ as follow: $B = - 596.52 a_{eff} + 393.4$, where B is in GPa, and $a_{eff}$ in nm. We found also that the bulk modulus B increases almost linearly with the increase of the melting point $T_m$ as follow: $B = 0.084 T_m - 38.12$. The average error on the estimation of B was found at around 10%.
We studied also the dependence between the Debye temperature $\theta_D$ and the effective cubic lattice constant $a_{eff}$ of our materials of interest. The Debye temperature $\theta_D$ decreases exponentially with the increase of the effective cubic lattice constant $a_{eff}$ as follow: $\theta_D = 165.46 + 3.8 \exp(-57.2\ a_{eff})$. The average errors on the estimation of $\theta_D$ was only around 4.5% from $\theta_D = 165.46 + 3.8 \exp(-57.2\ a_{eff})$ model, and around 1% from $\theta_D = - 416.5 + 879.8\ H - 434.4\ H^2 + 74.7\ H^3$ model, respectively.

## References


[1] X. He, and H. Shen, "First-principles study of elastic and thermo-physical properties of kesterite-type $Cu_2ZnSnS_4$", Physica B: Condensed Matter, Vol. 406, No. 24, (2011), pp. 4604–4607. https://doi.org/10.1016/j.physb.2011.09.035.

[2] S. Daoud, and A. Latreche, "Comment on density functional investigation on electronic structure and elastic properties of BeX at high pressure", Indian Journal of Physics: Vol. 90, No.11, (2016), pp.1243-1244. https://doi.org/10.1007/s12648-016-0863-4.

[3] H. Rekab-Djabri, M. M. Abdus Salam, S. Daoud, M. Drief, Y. Guermit, and S. Louhibi-Fasla, " Ground state parameters, electronic properties and elastic constants of $CaMg_3$: DFT study", Journal of Magnesium and Alloys, Vol. 8, No.4, (2020), pp. 1166-1175. https://doi.org/10.1016/j.jma.2020.06.007.

[4] S. Daoud, "Comment on structural phase transition, electronic and elastic properties in TlX (X = N, P, As) compounds: Pressure-induced effects" Computational Materials Science, Vol. 111, No. 1, (2016), pp. 532 - 533. https://doi.org/10.1016/j.commatsci.2015.09.022.

[5] S. Daoud, "Sound velocities and thermal properties of BX (X=As, Sb) compounds", International Journal of Scientific World: Vol. 3, No.1, (2015), pp. 43-48. https://doi.org/10.14419/ijsw.v3i1.4039.

[6] H. Rekab-Djabri, R. Khatir, S. Louhibi-Fasla, I. Messaoudi, and H. Achour, "FPLMTO study of new phase changes in CuX (X= Cl, Br, I) compounds under hydrostatic pressure", Computational Condensed Matter, Vol. 10, No. 3, (2017), pp. 15-21. https://doi.org/10.1016/j.cocom.2016.04.003.

[7] S. Daoud, P. K. Saini, and H. Rekab-Djabri, "Elastic constants and optical phonon frequencies of BX (X= P, As, and Sb) semiconductors: Semi-empirical prediction", International Journal of Physical Research: Vol. 8, No.2, (2020), pp. 45-49. https://doi.org/10.14419/ijpr.v8i2.31001.

[8] S. Daoud, " Sound velocities and thermal properties of BeX (X=S, Se and Te) alkaline-earth chalcogenides", International Journal of Scientific World, Vol.5, No.1, (2017), pp. 9-12. https://doi.org/10.14419/ijpr.v8i2.31001.

[9] N. Bioud, X-W. Sun, S. Daoud, T. Song, R. Khenata, and S. Bin Omran," High-temperature and high-pressure physical properties of CuI with zinc-blende phase by a systematic *ab initio* investigation", Optik, Vol. 155, No. 2, (2018), pp. 17-25. https://doi.org/10.1016/j.ijleo.2017.11.006.

[10] J. Tan, G. Ji, X. Chen, L. Zhang, and Y. Wen, "The high-pressure phase transitions and vibrational properties of zinc-blende XTe (X = Zn, Cd, Hg): Performance of local-density-approximation density functional theory", Computational Materials Science, Vol. 48, No. 4, (2010), pp. 796-801. https://doi.org/10.1016/j.commatsci.2010.03.037.

[11] S. Daoud, N. Bioud, and N. Lebga, "Structural, elastic, piezoelectric and electronic properties of (B3) AlP compound under pressure", Journal of optoelectronics and advanced materials, Vol. 16, No. 1-2, (2014), pp. 207-214. https://joam.inoe.ro/articles/structural-elastic-piezoelectric-and-electronic-properties-of-b3-alp-compound-under-pressure/.

[12] S. Daoud, N. Bioud, N. Lebga, and R. Mezouar, "Optoelectronic and thermal properties of boron-bismuth compound", International Journal of Physical Research, Vol. 2, No. 2, (2014), pp27-34. https://doi.org/10.14419/ijpr.v2i2.2760.

[13] S. Daoud, "Simplified expressions for calculating Debye temperature and melting point of II-VI and III-V semiconductors", International Journal of Scientific World: Vol. 3, No.2, (2015), pp. 275-279. https://doi.org/10.14419/ijsw.v3i2.5314.

[14] S. Daoud, "Linear correlation between Debye temperature and lattice thermal conductivity in II-VI and III-V semiconductors", International Journal of Scientific World: Vol. 3, No. 2, (2015), pp. 216-220. https://doi.org/10.14419/ijsw.v3i2.4793.

[15] S. Daoud, "Empirical study of elastic properties of BX (X = As, Sb) materials", International Journal of Scientific World, Vol.3, No.1, (2015), pp. 37-42. https://doi.org/10.14419/ijsw.v3i1.4022.

[16] M. Quintero, E. Moreno, S. Alvarez, J. Marquina, C. Rincón, E. Quintero, P. Grima, J-A. Heano, and M. A. Macías, "Lattice parameter values and phase transitions for the $Cu_2$-II-IV-$S_4(Se_4)$ (II = Mn, Fe, Co; IV=Si, Ge, Sn) magnetic semiconductor compounds", Revista Latinoamericana de Metalurgia y Materiales, Vol. 34, No. 1, (2014), pp. 28-38. http://ve.scielo.org/pdf/rlmm/v34n1/art03.pdf

[17] S. Adachi, "Earth-Abundant Materials for Solar Cells", John Wiley & Sons Ltd, the atrium, Southern Gate, Chichester, West Sussex, Po19 8SQ, United Kingdom, (2015). ISBN 9781119052777 https://doi.org/10.1002/9781119052814.

[18] S. Daoud, H. Rekab-Djabri, and N. Beloufa, "Melting point and microhardness of $Cu_2$-II-IV-$VI_4$ compounds ", International Journal of Physical Research, Vol. 10, No. 1, (2022), pp. 53-54. https://www.sciencepubco.com/index.php/IJPR/article/download/31946/16796

[19] K. Ito, "Copper Zinc Tin Sulfide-Based Thin-Film Solar Cells", John Wiley & Sons Ltd, the atrium, Southern Gate, Chichester, West Sussex, Po19 8SQ, United Kingdom, (2015). ISBN 978-1-118-43787-2 https://doi.org/10.1002/9781118437865.

[20] R. Mezouar, N. Bioud, and A. Benmakhlouf, "Correlation trend between the bulk modulus, microhardness and the lattice parameter of III-V semiconductors", International Journal of Advanced Chemistry, Vol. 10, No. 1, (2022), pp. 9-11. https://www.sciencepubco.com/index.php/IJAC/article/view/32020

[21] R.B.V. Chalapathy, G. S. Jung, and B. T. Ahn, "Fabrication of $Cu_2ZnSnS_4$ films by sulfurization of Cu/ZnSn/Cu precursor layers in sulfur atmosphere for solar cells", Solar Energy Materials & Solar Cells, Vol. 95, No.12, (2011), pp. 3216–3221. https://doi.org/10.1016/j.solmat.2011.07.017.

[22] Y. L. Gao, and Y. J. Dong, "Structural, mechanical and thermal properties of $Cu_2ZnSiS_4$ with four structures from the first-principle calculations", International Journal of Modern Physics B, Vol. 33, No. 9, (2019), pp. 1950067 (10 pages). https://doi.org/10.1142/S021797921950067X.

[23] Y. L. Gao, W. S. Guan, and Y. J. Dong. "Elastic and thermal properties of orthorhombic and tetragonal phases of $Cu_2ZnSiSe_4$ by first principles calculations". Semiconductors, Vol. 54, No. 10, (2020), pp. 1185–1190. https://doi.org/10.1134/S1063782620100115.

[24] S. Hasan, K. Baral, N. Li, and W-Y. Ching, "Structural and physical properties of 99 complex bulk chalcogenides crystals using frst-principles calculations", Scientific Reports, Vol. 11, (2021), pp. 9921 (18 pages). https://doi.org/10.1038/s41598-021-89281-6.

[25] A. Latreche and S. Daoud "Comment on pressure induced phase transition, elastic and thermal properties of rare earth tellurides", Transactions of the Indian Institute of Metals: Vol. 70, No.4, (2017), pp. 1159 -1160. https://doi.org/10.1007/s12666-016-0969-6.

[26] N. Bioud, "Comment on structural, electronic, elastic, optical and thermodynamic properties of copper halides CuCl, CuBr and their ternary alloys $CuCl_{1-x}Br_x$ $(0.0 \leq x \leq 1.0)$ using full-potential linear muffin-tin orbital (FP-LMTO) method [Optik 127 (2016) 4559-4573]", Optik, Vol. 127, No.23, (2016), pp. 11395-11397. https://doi.org/10.1016/j.ijleo.2016.08.020.

[27] K. Tang, T. Wang, W. Qi, and Y. Li, "Debye temperature for binary alloys and its relationship with cohesive energy", Physica B: Condensed Matter, Vol. 531, No.2, (2018), pp. 95–101.https://doi.org/10.1016/j.physb.2017.12.025.

[28] S. Daoud, N. Bioud, L. Belagraa, and N. Lebga, "Elastic, optoelectronic and thermal properties of boron phosphide", Journal of Nano-and Electronic Physics, Vol. 5, No.4, (2013), pp. 04061 (6pp). https://jnep.sumdu.edu.ua/download/numbers/2013/4/articles/jnep_2013_V5_04061.pdf

[29] G. Sai Gautam, and K.C. Hari Kumar, " Elastic, thermochemical and thermophysical properties of rock salt-type transition metal carbides and nitrides: A first principles study", Journal of Alloys and Compounds, Vol. 587, No. 2, (2014), pp. 380-386. https://doi.org/10.1016/j.jallcom.2013.10.156.

[30] S. Daoud, N. Bioud, L. Belagraa, and N. Lebga, "Corrigendum to the Manuscript Entitled "Elastic, Optoelectronic and Thermal Properties of Boron Phosphide" [J. Nano- Electron. Phys. 5 No 4, 04061 (2013)]", Journal of Nano-and Electronic Physics: Vol. 14, No.2, (2022), pp. 02030 (1pp). https://doi.org/10.21272/jnep.14(2).02030.