Regular article

FPLMTO study of new phase changes in CuX (X = Cl, Br, I) compounds under hydrostatic pressure

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ARTICLE INFO

ABSTRACT

We study the ground-state properties of copper halides CuX (X = Cl, Br, I) and the behavior under pressure using a recent version of the full potential linear muffin-tin orbitals method (FPLMTO). It predicts the possibility of an additional local minimum in the tetragonal PbO phase for CuBr and CuI at 0.7 GPa and 01.53 GPa with a direct energy gap at Γ of about 0.678 eV and 1.265 eV respectively. The use of GGA in this work is more appropriate than LDA and correctly predicts the cubic B3 phase as ground state structure for the three binaries. Importantly, calculated transition pressure Pt revealed also the presence of PbO phase at 5.333 GPa for CuCl which is consistent with experimental reports. Other important results are that concerned with the possibility of phase transition from B3 to the hexagonal B8 phase at lower pressures (3.43, 4.11 and 6.23) GPa and from B3 to B2 at (22.96, 22.66 and 24.83) GPa respectively for CuBr, CuI and CuCl.

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1. Introduction

There is a continuous interest in the study of the structural and electronic properties of high-pressure modification of I—VII CuI, CuCl and CuBr copper halides, due to their unusual properties compared to IV—IV, III—V and II—VI binaries [1—8]. In particular the strong p—d hybridization separates the copper halides from the other compounds. These materials are known to be semiconductors with a large and direct gap in their zinc-blende (B3) ground state phase and form the end of the class of tetrahedrally coordinated semiconductors. Further, early experimental studies suggest that under pressure CuCl, CuBr and CuI undergo a number of structural phase transitions for which it is known that high pressure can transform them from the zinc blende (B3) phase to the rocksalt (B1) phase [6,9,10,12]. In Previous works we have confirmed the possibility of a low-pressure phase transition from the zinc blende (B3) structure to the cubic CsCl (B2) structure [11]. However, only ZB, NaCl, CsCl and wurtzite phases of our compounds have been taken into account with FPLMTO method, using (LDA) approximation. Moreover, this theoretical investigation has been done to study the superlattice (SL) properties of these materials. Other works have

applied the FP-LAPW method in two main structures B1 and B3 to study the effect of pressure on the structural, elastic, and opto-electronic properties of these compounds. Authors show that calculations with GGA approximation are more appropriate than LDA and give a good description of structural properties of copper halides [9]. On the other hand, the experiments have shown the presence of a tetragonal structure for CuI, CuCl and CuBr at low temperature for pressures above 5 GPa. A. Blacha and al [12] assumed that this phase has PbO structure. However, it seems to be well established only for CuI and CuCl compounds. The phase diagram of CuBr was only partially known [12]. One of the purposes of the present work is to investigate this problem independent of the temperature and to calculate the pressure which induces the phase transition from B3 to B10 and to intermediate structures of lower symmetry. To the best of our knowledge no previous work was done on theoretical calculations exploring this problem, since it appears from literature that most of the works which addressed the ground state phase problem have focused only on the B3 and the B1structures. We have also investigated the electronic structure of copper halides for both the ground state B3 phase and the PbO (B10) phase. The paper is organized as follows: Section 2 describes the method, Section 3 is dedicated to the description of the results and Section 4 is for the conclusion.

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Table 1
Number of plane wave (PW), energy cut off (in Ry) and the muffin-tin radius (RMT) used in the calculation.

Structure	PW						$E_{cut}tot(Ry)$						RMT(u.a)							
	CuCl		CuBr		CuI		CuCl		CuBr		CuI		Cu		Cl		Br		I	
	LDA	GGA	LDA	GGA	LDA	GGA	LDA	GGA	LDA	GGA	LDA	GGA	LDA	GGA	LDA	GGA	LDA	GGA	LDA	GGA
NaCl (B1)	180	180	180	180	228	180	14.3	13.3	12.9	12.9	12.6	13.3	2.29	2.38	2.39	2.48	2.57	2.66	2.82	2.93
CsCl (B2)	163	163	163	163	215	215	11.0	12.1	12.3	12.8	11.1	11	2.41	2.15	2.1	2.01	2.31	2.41	2.01	2.3
ZB (B3)	306	306	228	228	228	228	15.3	14.3	12.5	17.1	11	14.3	2.32	2.31	2.32	2.4	2.41	2.41	3.02	2.40
Wz (B4)	524	524	686	686	390	390	12.2	12.4	37.2	37.2	9.1	12.4	2.36	2.36	2.36	2.31	1.64	1.64	2.83	2.43
NiAs (B8)	146	146	178	178	136	136	10.7	9.6	17.5	13.5	21.7	33.1	2.63	2.77	2.63	2.77	2.38	2.38	1.84	1.93
PbO (B10)	432	432	546	546	310	310	13.7	13.8	28.6	20.6	9.82	13.8	2.80	2.31	2.80	2.41	1.87	1.87	2.78	2.41

2. Method of calculation

The calculations were made using the all-electron full potential linear muffin-tin orbital (FPLMTO) augmented by a plane-wave basis (PLW) [13], within the framework of density functional theory (DFT) [14,15]. At the reverse of the previous LMTO methods, the present one treats the interstitial regions on the same footing with the core regions [13]. The exchange correlation energy of electrons is described in both the local density approximation (LDA) [14,15] and the generalized gradient approximation (GGA96) using the parameterization of Perdew and al [16,17]. In the FPLMTO, the non-overlapping muffin tin spheres MTS potential is expanded in spherical harmonics inside the spheres of radius RMTS. In the interstitial region, the s, p and d basis functions are expanded in a number (NPLW) of plane waves determined automatically by the cut-off energies. The available computer code lmtART [18,19] was used in the present work. In all cases, the maximal angular momentum for the expansion of the charge density and the potential in spherical harmonics was fixed to lmax = 6. The muffin-tin radius (RMT) values, number of plane waves (PW) and the total cut-off/energies used in our calculation, are listed in Table 1. Notice that the RMTS can be different for each atomic species in different phases since the full potential ensures the no dependency of calculations on the RMTS.

3. Results and discussion

3.1. Structural phase stability

In this paper, we report first principles total energy calculations to investigate the structural properties and phase transitions of copper halides under high-pressure. Several possible structural phases including NaCl (B1), CsCl (B2), ZB (B3), WZ (B4), NiAs (B8), and PbO (B10) structures have been considered in our calculations. Using the minimization curves, the equilibrium volume, the equilibrium lattice constant, the bulk modulus B and its derivative have been calculated by fitting to the numerical data to the usual Birch's equation of states (EOS) [20]. The NaCl, CsCl, ZB structures have cubic symmetry, so, unit cell volume depends on one parameter only, the lattice constant. For wurtzite, NiAs phases having

hexagonal symmetry, PbO (B10) having tetragonal symmetry we had to optimize lattice constants (i.e. a, c/a and b/a ratio) and internal parameters (u). Table 2 represents the position of atoms for each structure and the results are summarized in Table 4. It is clearly seen that for our three compounds the GGA overestimates the lattice parameters while the LDA underestimates it. Our GGA results are in reasonable agreement with literature. To the best of our knowledge, there are no data available for structural properties of copper halides in NiAs (B8) phase and in PbO (B10) phase at T = 0 °K. It is seen that the B8 structure has the highest bulk modulus value; this suggests that NiAs phase is more compressible than the other phases.

The stability of any particular structure corresponds to the lowest Gibbs free energy, which is given by $G = E + PV - TS$, where E is the internal energy, S represents the vibrational entropy, P is the given pressure and V stands for the volume. Since we performed the calculations at T = 0 °K, the Gibbs free energy G is then equivalent to the enthalpy $H = E + PV$ and the pressure Pt for which Gibbs energies of two phases are equal is defined as the transition between these two phases.

In Fig. 1a, b and c, we show the minimization curves for the different phases for the three compounds. Volume and energy are per single formula unit. Our calculations show controversial results for the tetragonal (B10) phase. In Fig. 1a and b, for CuBr and CuI compounds, LDA combined with PLW-FPLMTO shows that the ground state configuration is the PbO (B10) structure. In contrast the results with GGA96 approximation give ZB (B3) as the ground state phase with a minimum close to that of PbO (B10) phase. The difference between them is found to be so small 0.01077 and 0.00566 and eV (unit cell) $^{-1}$ respectively, so that we expect the B10 to be a metastable phase. We have checked our results by modifying our input parameters in such a way to improve our calculations but the results remained approximately the same. Thus, we are encouraged to predict the B10 phase is at least a metastable phase for CuBr and CuI and should present a second local minimum. The GGA calculations are here to strength this finding.

It is known that the LDA uses the exchange correlation density of the uniform electron gas of the same charge density at every point in the system regardless of the inhomogeneity of the real charge

Table 2
Location of atoms for each structure.

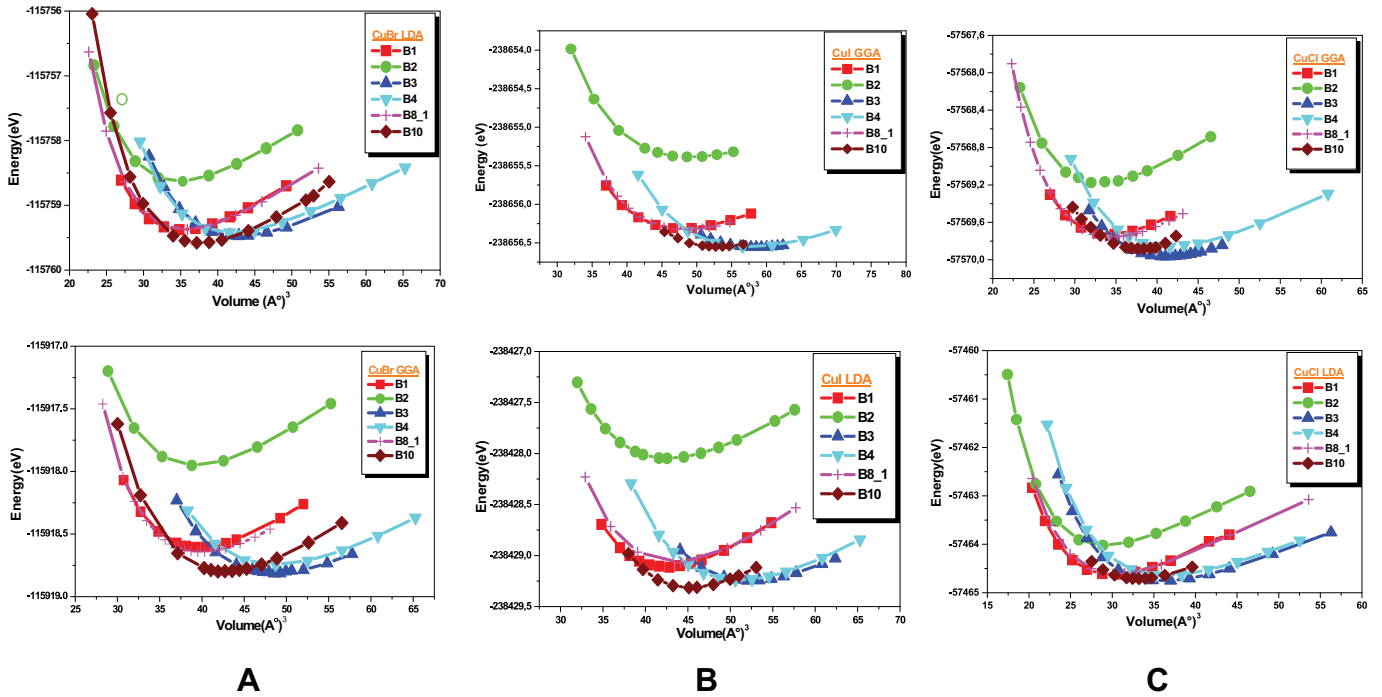|	Cu		Cl, Br, I	
	1st atom	2nd atom	1st atom	2nd atom
NaCl (B1)	0.0; 0.0; 0.0		1/2; 1/2; 1/2	
CsCl (B2)	0.0; 0.0; 0.0		1/2; 1/2; 1/2	
ZB (B3)	0.0; 0.0; 0.0		1/4; 1/4; 1/4	
Wz (B4)	0.0; 0.0; 0.0	$1.2; -1/2\sqrt{3}; 1/2$	0.0; 0.0; u	$1.2; -1/2\sqrt{3}; (0.5 + u)$
NiAs (B8)	0.0; 0.0; 0.0	0.0; 0.0; 1/2	$1.2; 1/\sqrt{12}; 1/4$	$1.2; -1/\sqrt{12}; 3/4$
PbO (B10)	3/4; 1/4; 0.0	1/4; 3/4; 0.0	1/4; 1/4; +z	3/4; 3/4; −z

Fig. 1. a: Variation of total energy with unit cell volume for six possible candidate structures of CuBr crystal. **b**: Variation of total energy with unit cell volume for six possible candidate structures of CuI crystal. **c**: Variation of total energy with unit cell volume for six possible candidate structures of CuCl crystal.

density. The general gradient approximation (GGA) also uses the gradient of the charge density to correct for this deviation, and therefore it is thought to be more accurate. On the other hand, our LDA approximation diagram in Fig. 1c shows for CuCl that the

ground state configuration is the PbO (B10) phase structure while the GGA calculations shows zincblende (B3) as ground state for this compound. So it is clearly seen that the GGA calculations correctly predicts the B3 structure as ground state structure for these binary

Table 3
Calculated values of the transition pressure Pt and transition volumes for CuBr CuCl and CuI compared to the other works.

Phases	Volume						Pression(GPa)								
	CuBr		CuCl		CuI		CuBr			CuCl			CuI		
	V ($A°$)³	Reduct (%)	V ($A°$)³	Reduct (%)	V ($A°$)³	Reduct (%)	Present work	Other works		Present work	Other works		Present work	Other works	
								Teo	Exp		Teo	Exp		Teo	Exp
B3→B1	V_{B3} 48.64 V_{B1} 39.76	18.25	V_{B3} 41.14 V_{B1} 47.49	17.01	V_{B3} 55.80 V_{B1} 39.76	28.74	4.25	3.69[h] 1.88[a]	6.4 −8.5[i]	06.55	08.7[g] 6.35[h]	8.8[c], 08.2[e]	03.93	2.29[e] 8.11[j]	8.0[e, f] 7.5[d] >9.69[b]
B3→B2	V_{B3} 48.64 V_{B2} 39.09	19.63	V_{B3} 41.14 V_{B2} 33.05	19.66	V_{B3} 55.80 V_{B2} 49.10	12.00	22.96		18.53[a]	24.83	22.32[a]		22.66	24.62[a]	
B3→B8	V_{B3} 48.64 V_{B81} 39.91	17.94	V_{B3} 41.14 V_{B81} 34.58	15.94	V_{B3} 55.80 V_{B81} 46.96	15.84	3.43			06.23			04.11		
B3→B10	V_{B3} 48.64 V_{B10} 42.92	11.75	V_{B3} 41.14 V_{B10} 38.036	07.54	V_{B3} 55.80 V_{B10} 52.98	05.05	0.7			5.333			01.53		

[a] Ref. [11].
[b] Ref. [28].
[c] Ref. [27].
[d] Ref. [12].
[e] Ref. [25].
[f] Ref. [29].
[g] Ref. [3].
[h] Ref. [7].
[i] Ref. [26].
[j] Ref. [9].

Table 4

Calculated structural parameters, equilibrium lattice constants a, structural parameter c/a, internal parameter u, bulk modulus B_0 and their first derivatives B'_0 for different phases analyzed for CuCl, CuBr, and CuI.

Parameters			NaCl (B1)		CsCl (B2)		ZB(B3)		WZ (B4)		NiAs(B8_1)		PbO(B10)	
			LDA	GGA	LDA	GGA	LDA	GGA	LDA	GGA	LDA	GGA	LDA	GGA
CuCl														
$V_0(Å^3)$	This Work		30.585	34.148	29,787	33,053	36.237	41.149	36.461	41.522	31.182	34.587	34.937	38.036
	Otherwork	theo	30.0607[a]		29.0147[a]		36.3388[a]		38.0569[a]					
		Exp												
a_0 (Å)	This Work		4.964	5.150	3099	3209	5.252	5.480	3.733	3.891	3.533	3.735	3.813	3.981
	Otherwork	theo	4.948[b], 5.156[b],		3.0728[a]		5.246[b], 5.455[b], 5.2578[a]		3.7701[a]					
			4.9357[a], 4.96[c], 5.021[d],											
		Exp	4.929[e]				5.424[e]							
B_0 (Gpa)	This Work		68.110	55,165	71,200	53,841	62.814	45.456	68.257	44.426	76.201	57.077	67.228	52.370
	Otherwork	theo	90.29[b], 59.05[b], 92.7[d],		96.5026[a]		76.787[b], 48.38[b]		69.8761[a]					
			80.3[d]				68.9934[a],							
							39.8[i], 54.5[j], 38.1[e]							
		Exp												
B'_0	This work		4.694	4.887	4428	4.909	4.806	4.284	4.647	6.662	4.999	4.413	4.655	4.927
	Otherwork	theo	5.142[b], 5.196[b], 4.9050[a]		4.4662[a]		5.195[b], 4.733[b] 5.0751[a] 4[a]		3.8967[a]					
		Exp	4[e]											
u	This Work								0.382	0.382				
									0.374[a]					
c/a	This Work								1.617	1.627	1.633	1.533	1.260	1.205
									1.64[a]					
z													0.272	0.286
CuBr														
$V_0(Å^3)$	This Work		35.848	39.76	34,889	39,094	43.193	48.649	42.965	47.914	35.806	39.917	38.518	42.928
	Otherwork	theo	35.1024[a]		34.3882[a]		44.0548[a]		44,7080[a]					
		Exp												
a_0 (Å)	This Work		5.234	5.418	3267	3393	5.569	5.794	3.939	4.086	3.711	3.929	3.901	4.053
	Otherwork	theo	5.207[b], 5.417[b]		3.2518[a]		5.530[b], 5.744[b]		3.9797[a]					
			5.1975[a],5.1425[g],.				5.60[a], 5.732[f],							
		Exp	5.1701[e]				5.695[e]							
B_0 (Gpa)	This Work		64.138	48.398	55,753	45,014	54.576	37.953	59.43	56.195	69.287	49.869	71.052	52.958
	Otherwork	theo	78.252[b]51.592[b],		80.1736[a]		66.822[b], 43.528[b]		60.7554[a]					
							64.3892[a]							
		Exp	84[e]				36.6[e]							
B'_0	This Work		4.468	4.968	5088	5.339	4.573	4.742	5.549	5.807	4.640	5.224	4.595	3.723
	Otherwork	theo	5.188[b], 4.977[b],		4.0713[a]		4.567[b] 5.1[b]		4.2495[a]					
			4.7621[a]6[g].				4.3620[a]							
		Exp												
u									0.382	0.382				
									0.374[a]					
c/a									1.623	1.621	1.618	1.520	1.297	1.289
									1.638[a]					
z													0.294	0.297
CuI														
$V_0(Å^3)$	This Work		42.448	47.798	42,349	49,107	52.294	55.80	61.420	68.947	32.920	46.964	39.830	52.986
	Otherwork	theo	42.6806[a]		42.5729[a]		52.4713[a]		54.8365[a]					
		Exp												
a_0 (Å)	This Work		5.537	5.760	3485	3661	5.936	6.066	4.458	4.598	3.624	4.180	4.028	4.345
	Otherwork	theo	5.530[b], 5.744[b], 5.54[a],		3.49[a]		5.885[b] 6.097[b], 5.94[a]		4.26[a]					
			6.082[f]											
		Exp												
B_0 (Gpa)	This Work		65.48	42.22	56,342	31,186	51.193	34.864	51.193	37.776	66.051	42.955	52.170	40.425
	Otherwork	theo	69.1603[b], 46.116[b]		56.7835[a]		58.483[g]		54.72[a]					
		Exp					36.6[e], 31[h]							
B'_0	This Work		5.262	5.015	4238	4.5973	5.226	5.033	4.878	4.425	4.725	4.733	5.280	5.521
	Otherwork	theo	4.677[b], 4.672[b]		4.1086[a]		4.737[b], 4.704[b]		4.13a					
		Exp					4b[a]							
u									0.382	0.382				
									0.374[a]					
c/a									1.601	1.638	1.597	1.485	1.219	1.291
z													0.276	0.289

[a] Ref. [11].
[b] Ref. [9].
[c] Ref. [5].
[d] Ref. [3].
[e] Ref. [10].
[f] Ref. [21].
[g] Ref. [22].
[h] Ref. [23].
[i] Ref. [24].
[j] Ref. [25].

compounds, and it is expected that pressure can transform them to B10, B8, B1 and B2 structure.

3.2. Structural phase transition

The calculated values of Pt are listed in Table 3 with the volume reduction for each transition, and we display in Fig. 2a, b and c, for the three compounds, the enthalpy differences for B1, B2, B10 and B8 phases as a function of pressure with reference to B3. In agreement with the experiment, the obtained results show that CuI and CuCl undergo a number of structural phase transitions under pressure. The new phase transition (B3−B8) is predicted to occur before the known phase transition (B3−B1) at 04.11 and 06.23 GPa. And the two structures (B1−B8) appear to be degenerate with the energy differences of 0.01465 and 0.02899 eV for the two compounds respectively. On the other hand the (B3−B10) phase transition is predicted to occur at 01.53 and 5.333 GPa. So the B10 phase should present a second local minimum for CuI. It is clearly seen that our results confirm the presence of tetragonal PbO phase under low pressure at T = 0 °K, which is consistent with previous experimental and theoretical reports at low temperature [12]. Our results for B3−B1 transition agree well with experimental and other calculated values.

We have calculated the structure transition pressure for CuBr, from B3 to B8 phase as 3.43 GPa, and from B3 to B1 at 4.25 GPa. The case of transition pressure from B3 to the metastable B10 structure is of particular interest because the phase diagram of tetragonal phase to be assumed as B10 phase in Ref. [12] was only partially known. Our result phase transition from B3 to the B10 structure was found to occur at 0.7 GPa. It can be seen that there is about 17.94, 18.25 and 11.75% volume reduction for B3−B8, B3−B1 and B3−B10 phase transitions respectively. To the best of our knowledge there are no experimental or theoretical data in literature with the consideration of constant-temperature limit to compare our results for the pressures, which induce phase transitions from B3 to B10 and to B8. We have also calculated for CuBr the energy differences between B1−B8 structures as 0.03624 eV.

Our results for B3−B2 transition pressure are 22.96, 24.83 and 22.66 GPa respectively for CuBr CuCl and CuI. Likewise, no GGA theoretical values and experimental data have been reported so far, regarding these phase transitions.

In all cases, the wurtzite (B4) phase is close to the zinc-blende (B3) phase for the three compounds especially for CuI where the difference is 0.0042 eV only. In fact, Wurtzite and zinc blend are structurally similar, they differ only by the stacking in the (1 1 1) direction.

Other, structures have been considered in our calculations but were not closed to stability in any range of pressures of interest.

3.3. Electronic properties

We have calculated the band structures of copper halides in B3 and B10 phases using the FPLMTO-PLW with the GGA approaches. It is very clear that B3 and B10 phases are direct-band gap at Γ point for the three compounds. Results for the gaps are summarized in Table 5. In Fig. 3a and b, we have shown the band structure of CuBr, CuCl and CuI in the two phases. For B10 phase, we remark a large and direct fundamental gap Eg of about 0.678, 0.697 and 1.265 eV respectively for the three compounds with both the top of VB and the bottom of CB located at Γ.Our results for CuCl and CuI are consistent with the experiment reports and Ref. [12] calculations at low temperature for pressures above 5 GPa. In effect, authors suggest that the lowest-energy gap of the B10 phase of these two compounds should be direct at Γ point. However, There are no experimental results available to us to check our results at T = 0 °K.
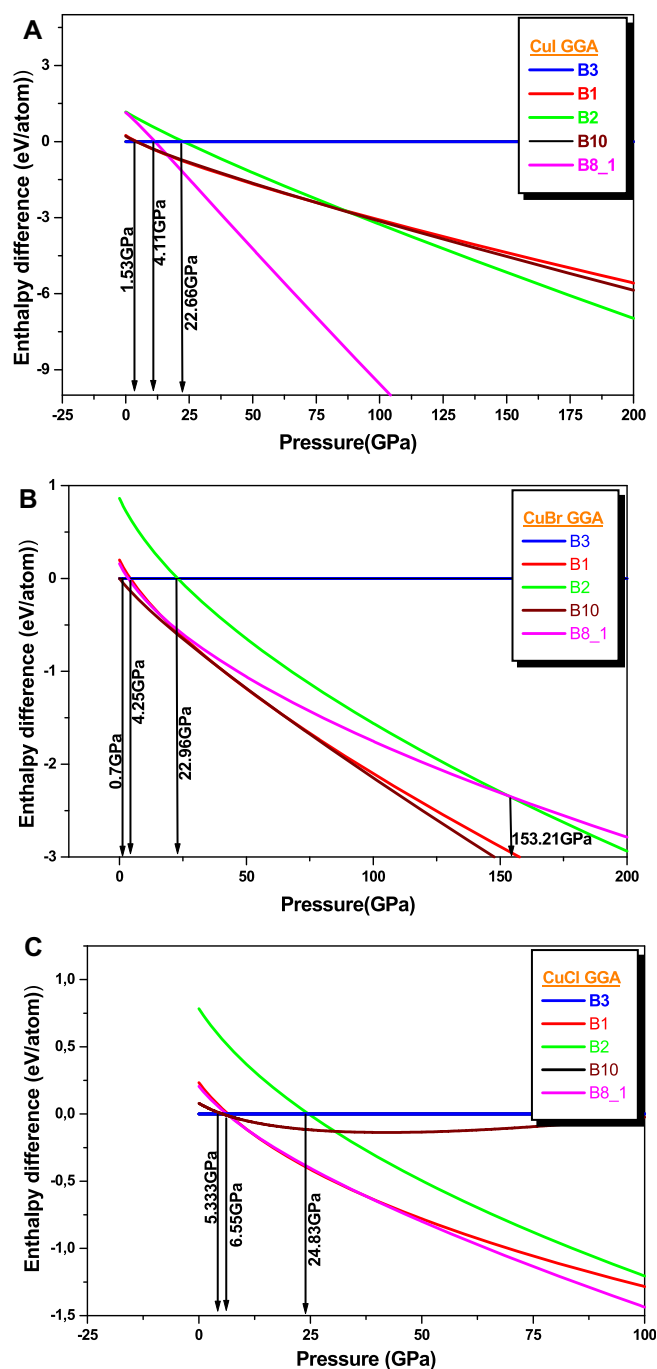

Fig. 2. a: Variation of the enthalpy differences DH (Ry) versus pressure (GPa) for NaCl (B1), CsCl (B2), ZB (B3), NiAs (B8) and PbO (B10) phases of CuI. The reference Gibbs free energy in set for B3 phase. **b**: Variation of the enthalpy differences DH (Ry) versus pressure (GPa) for NaCl (B1), CsCl (B2), ZB (B3), NiAs (B8), and PbO (B10) phases of CuBr. The reference Gibbs free energy in set for B3 phase. **c**: Variation of the enthalpy differences DH (Ry) versus pressure (GPa) for NaCl (B1), CsCl (B2), ZB (B3), NiAs (B8), and PbO (B10) phases of CuCl. The reference Gibbs free energy in set for B3 phase.

Also, to the best of our knowledge the electronic properties for CuBr have not yet been measured or calculated, hence our results for the B10 phase can serve as a prediction for future investigations.

4. Conclusion

We have resorted to a recent version of the PLW-FPLMTO

Table 5
The gaps of CuCl, CuBr and CuI in ZB and PbO phases in eV.

Compounds	Structure	Gap	Eg in (eV)	type	Experimental results	Other calculations
CuBr	B3	$\Gamma \rightarrow \Gamma$	0.426	Direct	3.05[c]	0.418[e] 0.445[a]
	B10	$\Gamma \rightarrow \Gamma$	0.678	Direct	/	/
CuCl	B3	$\Gamma \rightarrow \Gamma$	0.605	Direct	3.40[b]	0.509[e]0.538[a]
	B10	$\Gamma \rightarrow \Gamma$	0.697	Direct	2.90[d]	0.84[f]
CuI	B3	$\Gamma \rightarrow \Gamma$	1.027	Direct	2.95[d]	1.077[e] 1.118[a]
	B10	$\Gamma \rightarrow \Gamma$	1.265	Direct	2.92[d]	1.3[f]

[a] Ref. [30].
[b] Ref. [31].
[c] Ref. [32].
[d] Ref. [5].
[e] Ref. [9].
[f] Ref. [12].

Combined with both LDA and GGA96 for the calculation of the structural, phase stability and electronic properties of the copper halides CuBr, CuCl and CuI. The main results of the present work can be summarized as follows:

- The calculations predict the possibility of a second local minimum in the PbO (B10) phase for CuBr and CuI at 0.7 GPa and 1.53 GPa.
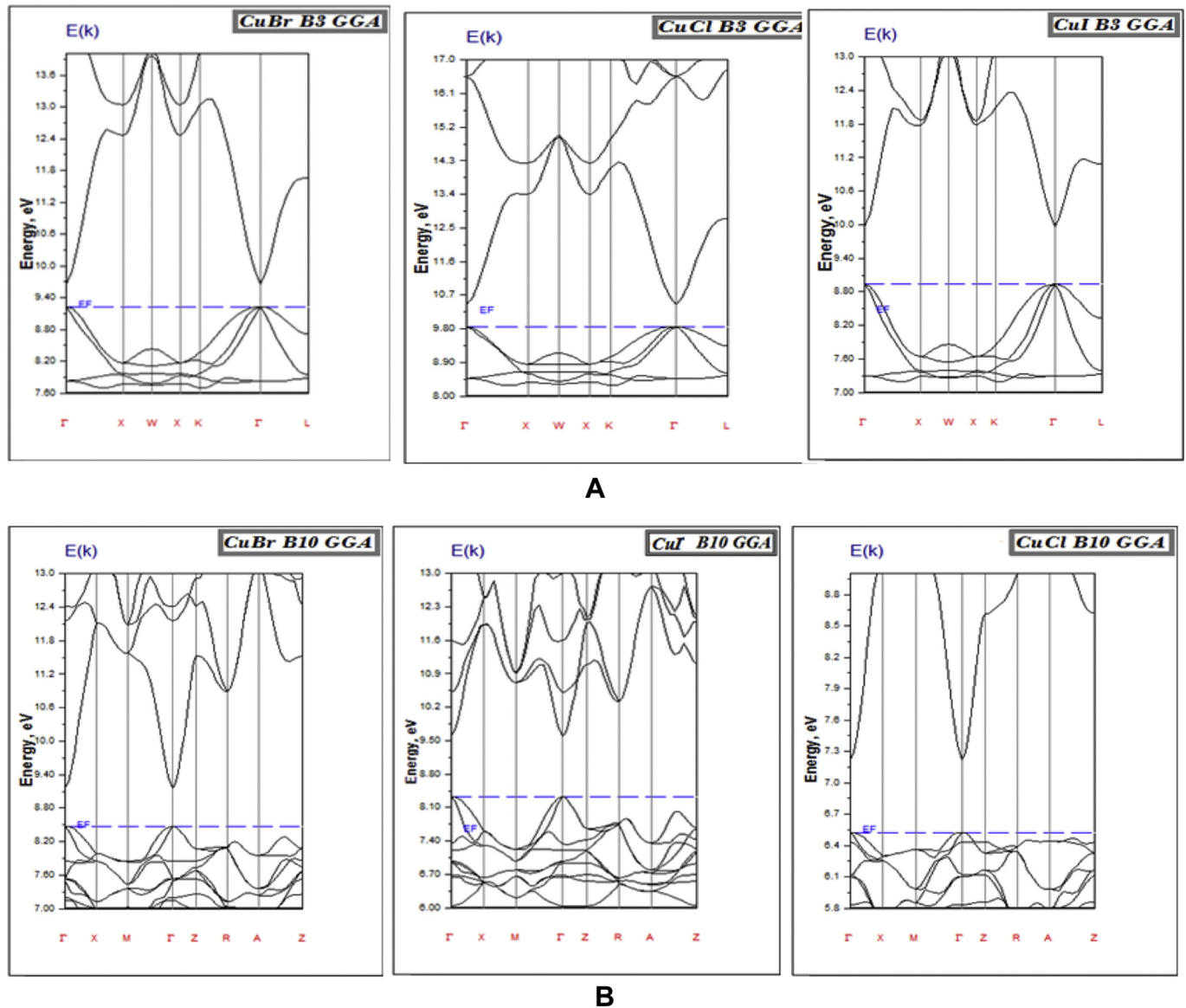

Fig. 3. a: Band structures of B3 phases of CuBr, CuCl and CuI. The energy zero is taken at Ef. **b**: Band structures of B10 phases of CuBr, CuCl and CuI. The energy zero is taken at Ef.

- The calculations clearly indicate that there is a structural transition from B3 to B10 at 5.333 GPa for CuCl confirming experimental suggestions.
- The results show that the GGA calculations correctly predict the ground state structure for our three binaries.
- We find that the B3 phase is slightly lower in energy than the B4 phase, and it transforms to the B8 new phase above (3.43, 04.11 and 06.23) GPa and also to B2 new phase at (22.96, 22.66 and 24.83) GPa respectively for CuBr CuI and CuCl.
- The transition pressure B3— B1 is in reasonable agreement with literature.

The electronic structure calculation for B10 phase at low pressures showed that the copper halides exhibit large and direct band gaps of 0.678, 1.265 and 0.697 eV respectively for CuBr CuI and CuCl.

Acknowledgements

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