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# Theoretical Investigation of Structural Properties of CuCl, CuBr and CuI Compounds under Hydrostatic Pressure

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**Abstract.** We have applied a recent version of the full potential linear muffin-tin orbitals method (FPLMTO) to study the structural properties of copper halides CuX (X=Cl, Br, I) under high pressure using the generalized gradient approximation (GGA) for the exchange and correlation potential by Perdew et al. Results are given for lattice parameters, bulk modulus and its first derivatives in the wurtzite (B4), zinc-blende (B3), CsCl (B2), rock-salt (B1), and PbO (B10) structures. The results of these calculations are compared with the available theoretical and experimental data.

**Keywords:** FPLMTO; structural properties; Copper halides; Phase transitions.

**PACS:** 71.15.Mb; 74.62.Fj; 71.20.Nr

## INTRODUCTION

The copper halides CuI, CuCl and CuBr in their bulk form present many unusual features compared to IV–IV, III–V and II–VI binaries [1-5]. In an attempt to help understand the bulk structural parameters of these materials in different phases, we report a detailed calculation of structural properties of these materials in the wurtzite(B4), zinc-blende (B3), CsCl (B2), rock-salt (B1), and PbO (B10) structures at zero temperature.

The calculations were made using the all-electron full potential linear muffin-tin orbital (FPLMTO) augmented by a plane-wave basis (PLW) [6]. The exchange-correlation energy of electrons is described in the generalized gradient approximation (GGA96) using the parameterization of Perdew et al [7]. The available computer code lmtART [6,8] was used in the present work.

## THEORETICAL FRAMEWORK

The details of calculations are the following. Both LMTO-basis set and charge density are expanded inside the muffin-tin spheres in spherical harmonic functions with cut-off  $l_{\max}$ , and in Fourier series in the interstitial region. In the muffin-tin spheres (MTS) of radius  $R_{MT}$ , the upper limit on the angular momentum expansion of

the smoothed Hankel functions about a given atomic site is carried out up to  $l_{\max}=6$ . 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. In order to achieve convergence of energy eigenvalues, the wave functions in the interstitial region are expanded in plane waves with a cutoff of  $R_{\text{MT}} \times K_{\text{MAX}}$  equal to 8, where  $K_{\text{MAX}}$  is the maximum modulus for the reciprocal lattice vector and  $R_{\text{MT}}$  is the average radius of the MT spheres.

## RESULTS AND DISCUSSION

Using the present FPLMTO for the three binaries compounds, we have calculated the equilibrium volume corresponding to the lowest total energy, the equilibrium lattice constants, the bulk modulus and its derivative by fitting the total energy as a function of volume to the Murnaghan equation of state [9]. The results are summarized in Table 1, and the total energy variations with volume for the different phases are displayed in figure 1, figure 2 and figure 3. Volume and energy are as per the single formula unit.

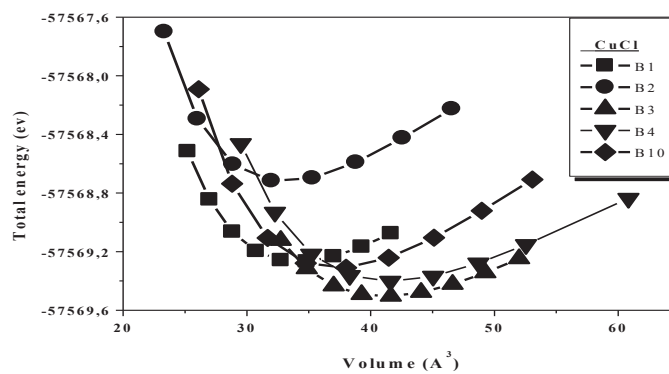


FIGURE 1. Calculated total energy versus relative volume for CuCl

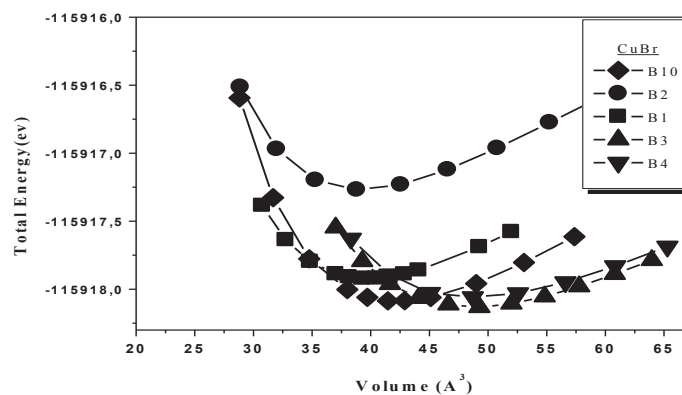
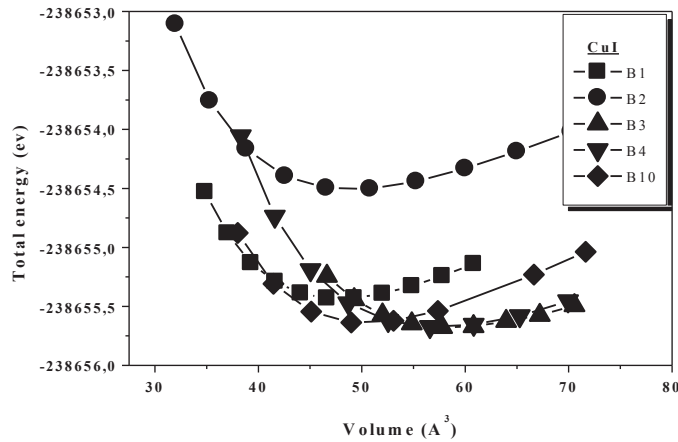


FIGURE 2. Calculated total energy versus relative volume for CuBr



**FIGURE 3.** Calculated total energy versus relative volume for CuI

**TABLE 1.** Calculated structural parameters equilibrium volumes  $V_0$  (in  $\text{\AA}^3$ ), lattice constants  $a$  (in  $\text{\AA}$ ), structural parameter  $c/a$ ,  $b/a$ , and the internal structural  $U$ , and bulk moduli  $B_0$  (in GPa) and their first derivatives  $B'_0$ , for B1, B2, B3, B4 and B10 phases.

\* Present work, <sup>a</sup>—Ref. 10, <sup>b</sup>—Ref. 11-with LDA, <sup>c</sup>—Ref. 11-with GGA, <sup>d</sup>—Ref. 12, <sup>e</sup>—Ref. 13, <sup>f</sup>—Ref. 14, <sup>g</sup>—Ref. 15, <sup>h</sup>—Ref. 16, <sup>i</sup>—Ref. 13, <sup>k</sup>—Ref. 16.

Parameters	B1	CsCl (B2)	Zb (B3)	WZ(B4)	PBO
<b>CuCl</b>					
$V_0(\text{\AA}^3)$	39.768*	39.093*	41.094*	41.623*	37.306*
$a_0(\text{\AA})$	5.152*5.156 <sup>k</sup>	3.393*	5.77*5.420 <sup>a</sup> 5.246 <sup>b</sup>	4.162*	3.575*
$B_0$ (GPa)	55.312* 59.05 <sup>k</sup>	45.014*	44.426*48.38 <sup>c</sup> 49 <sup>d</sup>	40.601*	54.724*
$B'_0$	4.680*4.733 <sup>k</sup>	5.340*	5.018*5.142 <sup>b</sup> 5.196 <sup>c</sup>	4.92*	4.806*
$U$				0.412*	
$c/a$				1.601*	1.633*
<b>CuBr</b>					
$V_0(\text{\AA}^3)$	39.766*	33.053*	48.702*	48.6.5*	42.352*
$a_0(\text{\AA})$	5.418*5.417 <sup>k</sup>	3.209*	5.797*5.744 <sup>c</sup> 5.732 <sup>d</sup>	4.382*	3.729*
$B_0$ (GPa)	48.398* 51.592 <sup>k</sup>	53.841*	37.806*36.6 <sup>a</sup>	37.218*	49.428*
$B'_0$	4.967*4.977 <sup>k</sup>	4.908*	4.754*4.567 <sup>b</sup>	5.299*	4.732*
$U$				0.382*	
$c/a$				1.601*	1.633*
<b>CuI</b>					
$V_0(\text{\AA}^3)$	47.798*	48.747*	47.798*	57.426*	50.436*
$a_0(\text{\AA})$	5.760*5.744 <sup>k</sup>	3.653*	5.760*5.885 <sup>b</sup>	4.598*	3.953*
$B_0$ (GPa)	57.69* 46.116 <sup>k</sup>	27.803*	42.219*39.7 <sup>d</sup>	37.776*	45.210*
$B'_0$	5.016*4.672 <sup>k</sup>	5.410*	5.015*4.704 <sup>c</sup>	4.425*	5.223*
$U$				0.422*	
$c/a$				1.638*	1.633*

To determine the most stable structure at finite pressure and temperature, we have used the enthalpy  $H=E+PV$  since we consider the temperature constant. Our calculations show that the ground state configuration phase for the three binaries is the

zinc-blende (B3) structure at ambient conditions. Nevertheless, depending on the pressure, these compounds, exhibit PbO, NaCl and CsCl from zinc-blende structures.

The results for the transition pressure from B3 to PbO structure for CuCl, CuBr and CuI are of 5.37GPa, 3.52 GPa and 4.20 GPa. We also report that for our three compounds respectively, a transition pressure from B3 to B2 occurs at 24.74 GPa, 20.38 GPa and 26.95 GPa. However, no theoretical values and experimental data have been reported so far to the best of our knowledge regarding these transitions. We notice for the transition pressure from B3 to B1 structure for the three compounds, a good agreement with literature. Our results for the three compounds respectively are 6.89 GPa, 5.97 GPa and 6.021 GPa.

## CONCLUSION

We have investigated the performance of a recent version of first principle technique FPLMTO combined with GGA96 for the calculation of the structural and phase stability properties of copper halides CuCl, CuBr and CuI. We confirm that the zinc-blende (B3) structure is the most stable at ambient pressure for the three binaries compounds. Depending on the pressure, these compounds, exhibit PbO, NaCl and CsCl from zinc-blende structures. In all cases, the wurtzite (B4) phase is close to the zinc-blende (B3) phase especially for CuI where the difference is 6.32meV only.

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## REFERENCES

1. A. Goldmann, Phys. Stat. Sol. B 81 (1977) 9.
2. S.F. Lin, W.E. Spicer, R.S. Bayer, Phys. Rev. B 14 (1976) 551.
3. J. Serrano, Ch. Schweitzer, K. Reimann, M. Cardona, D. Fro, Phys. Rev. B 65 (2002) 125110.
4. C.W. Cha, A.P. Ruskov, S. Huang, S. Early, C.Y. Huang, Phys. Rev. B 18 (1978) 2116.
5. S. Hule, D.A. Keen, Phys. Rev. B 50 (1994) 5868.
6. S.Y. Savrasov, Phys. Rev. B 54 (1996) 16470.
7. J.P. Perdew, Y. Wang, Phys. Rev. B 45 (1992) 13244.
8. [/http://www.physics.ucdavis.edu/mindlabS](http://www.physics.ucdavis.edu/mindlabS).
9. F.D. Murnaghan, *Proc. Natl. Acad. Sci. USA* 30 (1944) 5390.
10. S. Hull, D.A. Keen, Phys. Rev. B 50 (1994) 5868.
11. J.C. Marini, B. Stebe, E. Kartheuser, Phys. Rev. B 50 (1994) 14302.
12. Ali Zaoui, Fouad El Haj Hassan, *Philos. Mag.* B 82 (2002) 791.
13. V.Meisaloand M.Kalliomaki, *High Temp. High pressures* 5,663(1973).
14. H.C.Hsueh, J. R. Maclean, G. Y.Guo, G.J.Ackland, J Crain, *Phys. Rev. B* 51 (1995) 12216.
15. J. R. Chelikowsky, *Phys. Rev.* B35, (1987) 1174.
16. B. Amrani, T. Benmessabih, M. Tahiri, S. Hiadsi, F. Hamdache, *Physica B* 381 (2006) 179.