

Structural and Electronic Properties of the BN, BP and BAs in the Different Phases of Zinc-Blende, NaCl and CsCl

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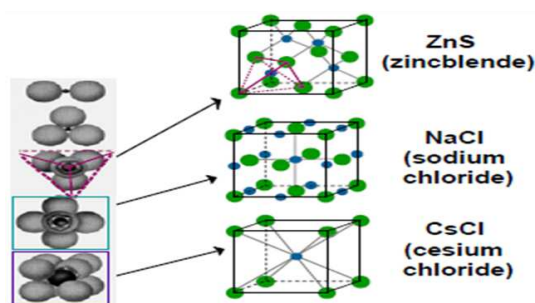
In this work we used the first *ab initio* calculations to study the stability of the binary alloys BN, BP and BAs and their behavior in the different phases of zinc-blende, NaCl and CsCl. The full potential linearized augmented plane wave method was employed within density functional theory. Our results show the difference in the calculated structural properties and the band structure is obtained for the zinc-blende structure. We have investigated the lattice parameters and band gap energies. We also give the valence charge density at a high pressure and the analysis of the density of states.

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PACS/topics: binary alloys, ab initio calculations, lattice parameter, high pressure, band-structure, charge density

1. Introduction

The boron-based compounds belong to the family of III–V semiconductors. These are compounds with a large gap, particularly interesting for their applications in the field of high temperatures and for the realization of opto-electronic components. The small core size of the boron atom B and the absence of *p* electrons explain their properties. Boron has a deep and localized pseudo potential compared to other atoms in the same column of the periodic table. The preliminary calculations of the ionicity [1, 2], illustrate these features. The compounds BP, BAs and BSb crystallize, meanwhile, in the zinc blende structure although there are many theoretical first-principle [3, 4] devoted to structural and electronic properties of BN, BP and BAs in their cubic phase, there are very few experimental data on these compounds [5, 6]. The fundamental properties (not the network to balance and rigidity modulus) and electronic properties of BN, BP and BAs were studied by Wentzcovitch et al. [7, 8] which also discussed the properties of these materials to high pressure [9].



2. Computational method

All of these studies are based on the local density approximation (LDA) associated with the density of functional theory (DFT). The self-energy is usually approximated using a perturbative expansion with respect to the quasi-particle interaction. The quantitative calculation of excitation energies in the binary alloys is the approximation GWA. In this approximation, the self-energy is the product of the single-particle Green function *G* and the screened interaction *W*. Hedin first proposed the GWA for the computation of quasiparticle energies in 1965. However, the approach was not applied to large-scale, numerical electronic structure calculations. The resulting band gaps compare much better with experiment. To provide estimates of cohesive energies of these compounds, Surh et al. [10] used the GW approximation to consider the effects of exchange and correlation of quasiparticles and recently, Rubio [11] made a calculation of the cubic phase of BN, we note the work of Ferhat et al. [12] and as well as Zaoui et al. [13]. We use the full potential linearized augmented plane wave (FP-LAPW) method implemented in the WIEN97 program [14] to study BN, BP and BAs in the zinc blende phase, NaCl (rocksalt) and CsCl. All of these studies is based on the LDA [15] associated with the theory of DFT [16, 17].

3. Results and discussion

Variation of the total energy versus atomic volume of BN, BP, and BAs for the different phases ZB, NaCl, and CsCl are shown in Figs. 1, 2, and 3 and it is obvious from these curves that the ZB structure is the most stable at ambient pressure, which is consistent with the experimental results. The corresponding equilibrium lattice parameter, bulk modulus and its pressure derivative are given in Tables I, II, and III for each compound for ZB,

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NaCl and CsCl structures. We see, from this table, that our calculated values are in better agreement with experiment than the other calculations. We confirm this result with the only existing one, which was recently performed by Zaoui and El Haj Hassan [18] using LDA within DFT and the pseudo potential method.

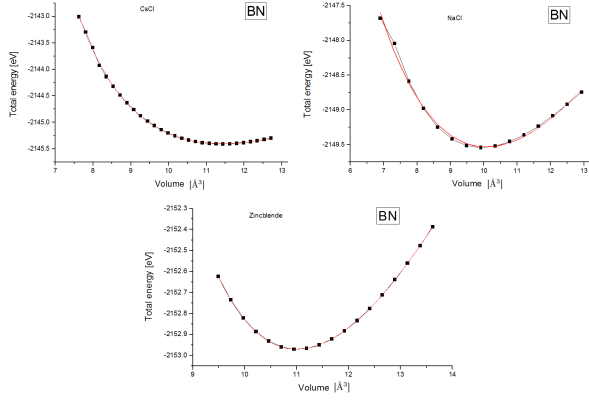


Fig. 1. Variation of the total energy versus volume atomic of BN for zinc blende, NaCl, and CsCl.

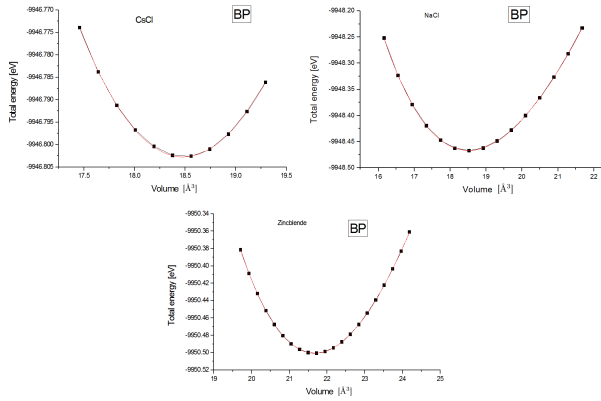


Fig. 2. Variation of the total energy versus volume atomic of BP for zinc blende, NaCl, and CsCl.

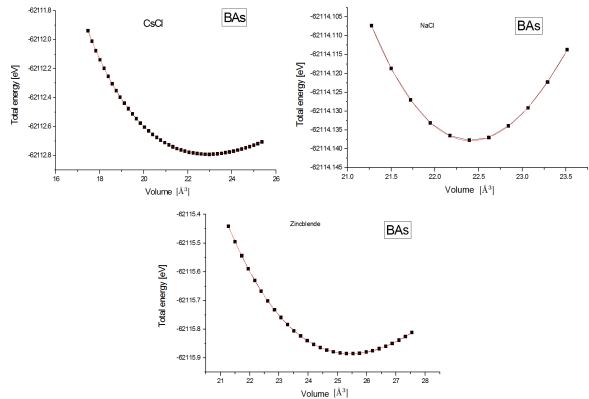


Fig. 3. Variation of the total energy versus volume atomic of BAs for zinc blende, NaCl, and CsCl.

TABLE I

Structural properties of BN for zinc blende, NaCl, and CsCl.

	Lattice [\AA]	B [GPa]	B'
Zinc blende			
calculations	3.530	417.44	3.78
experiment	3.615 [19,20,21]		
other calculations	3.606 [22]	367 [22]	
NaCl			
calculations	3.428	421.08	2.04
other calculations	3.493 [22]	425 [22]	
CsCl			
calculations	3.575	265.89	4.62

TABLE II

Structural properties of BP for zinc blende, NaCl, and CsCl.

	Lattice [\AA]	B [GPa]	B'
Zinc blende			
calculations	4.425	182.81	3.77
experiment	4.538 [20, 21]		
other calculations	4.558 [22]	166 [22]	
NaCl			
calculations	4.199	180.65	4.11
other calculations	4.339 [22]	155 [22]	
CsCl			
calculations	4.196	153.85	1.92

The band structure of BN, BP and BAs for ZB are shown in Fig. 4, respectively. The results are given in Table IV and show that BN is a direct-gap semiconductor with the minimum of conduction band at Γ , X point with energy gap 4.67 eV, and BP has an the indirect gap with minimum of conduction band at Γ , Δ_{\min} with energy gap 1.15 eV. The BAs has an indirect gap with minimum of conduction band at Γ , Δ_{\min} with energy gap 1.01 eV. There is a good agreement with experimental results. Valence charge density distribution in the zinc-blende structure at equilibrium volume for BN, BP, and BAs are given in Fig. 5.

TABLE III

Structural properties of BAs for zinc blende, NaCl, and CsCl.

	Lattice [\AA]	B [GPa]	B'
Zinc blende			
calculations	4.668	154.30	3.87
experiment	4.777 [21]		
other calculations	4.777 [22, 23]	145 [22]	
NaCl			
calculations	4.475	154.18	4.30
other calculations	4.583 [22]	143 [22]	
CsCl			
calculations	4.510	128.53	4.06

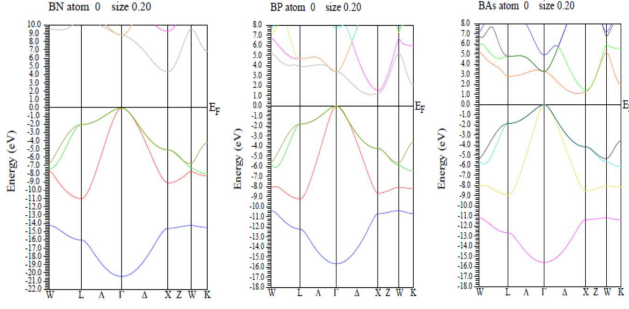


Fig. 4. Band-structures of zinc blende for the BN, BAs, and BP.

TABLE IV

Band gaps of BN, BP, and BAs in the zinc blende structure (all energies are in eV).

Compounds	Calculation	Other calculations
BN		
direct gap $\Gamma \rightarrow x$	4.67	4.19 [24], 4.40 [25], 4.24 [26], 4.6 [27]
BP		
indirect gap $\Gamma \rightarrow \Delta_{\min}$	1.15	1.2 [28], 1.9 [29], 1.14 [30]
BAs		
indirect gap $\Gamma \rightarrow \Delta_{\min}$	1.01	1.23 [13], 1.60 [30], 1.25 [23]

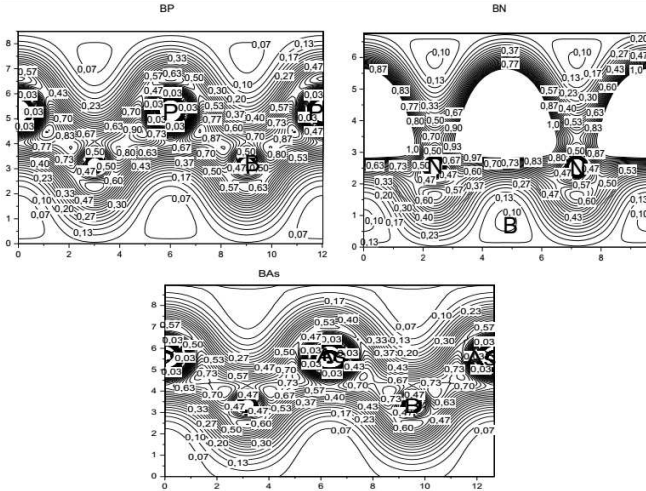


Fig. 5. Valence charge density distribution in the zinc blende structure at the equilibrium volume for BN, BP and BAs.

The charge contours are shown in the (110) plane, if we show the last closed contour as an indication of the size of the atom, at the transition volume for BN. The N atoms are much larger than the B atoms but for BP and BAs. The P and As atoms are much smaller than the B atoms. The total density of states and partial BP (zinc blende) at equilibrium is given in Fig. 6. We can distinguish, from the origin of energy two important valence regions

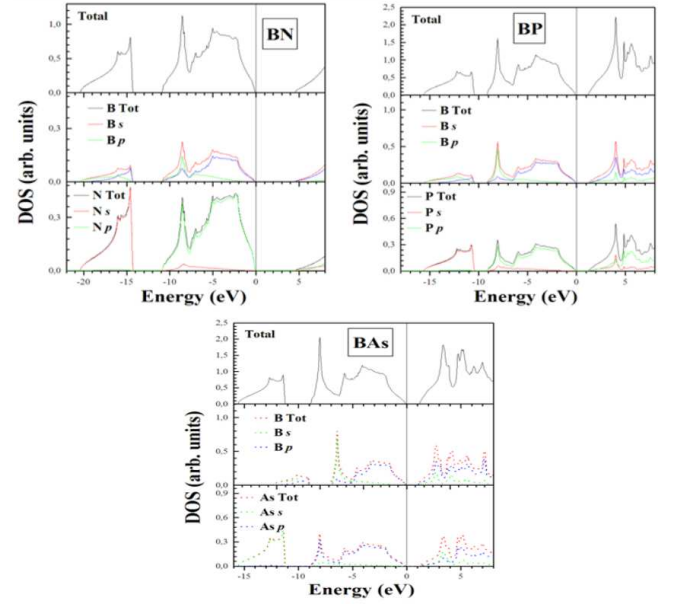


Fig. 6. States density distribution in the zinc blende structure at the equilibrium volume for BN, BP, and BAs.

called: VB1 and VB2. Hybridization is sp type with a strong participation of the p orbital in VB1 and s orbital in the VB2. The s orbital participation in the conduction band is less important than that of the p orbital.

4. Conclusion

This work is a contribution to the study of structural and electronic properties of the materials based on boron and copper by the method FP-LAPW. The boron-based compounds BN, BP, and BAs crystallize in the zinc blende structure. We studied the relative stability of phases NaCl (rock salt) and CsCl.

Our calculation of the electronic structure of BP and BAs indicates the presence of a fundamental indirect gap near X ($\Gamma \rightarrow \Delta_{\min}$), while for the BN we found a direct gap following ($\Gamma \rightarrow x$). These results agree with those of Wentzcovitch.

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