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First-principles study of zinc-blende to rocksalt phase transition in BP and BAs

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ABSTRACT

The structural and electronic properties of BP and BAs are investigated by first-principles pseudopotential method. The calculations show the structural phase transition from zinc-blende (ZB) structure to rocksalt (RS) structure at the transition pressure of 142 GPa for BP and 134 GPa for BAs. The ZB phase of BP and BAs remains indirect gaps upon applying hydrostatic pressure, while RS phase of BP and BAs is semimetal at the transition pressure.

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1. Introduction

Boron compounds have attracted increasing research interest over the past few years, as wide-gap semiconductors. These materials are of great technological interest for high temperature application and electro-optical devices in the short-wavelength range of the visible spectrum. This is due to their unique physical properties such as extremely high thermal conductivities, low dielectric, low densities, wide band-gap etc. In fact, the behavior of these compounds is truly unique among the IIIA–VA and IIB–VIA families. This originates from the absence of p electrons in the core of the B atom and its small size.

Under normal conditions, BP and BAs crystallize in the ZB structure. The experimental studies of the properties for these two compounds are very scarce due to the difficulties involving in its synthesis. Xia et al. [1] reported experimentally that ZB–BP did not undergo any transition up to at least 110 GPa, while ZB–BAs has been reported to transition into an amorphous state at a pressure of 125 GPa [2]. This amorphous state does not undergo any further transformation up to 165 GPa and persists as a metastable phase upon release of pressure. The pressure-induced amorphization of BAs was interpreted as an indication of the result of a kinetically frustrated ZB → RS transition by Green et al. [2]. Theoretical work on the high-pressure phases of BP and BAs has so far been limited to the study of the energetics of the RS, β-Sn and CsCl phases [3]. The RS phase was found to be marginally lower in enthalpy than the β-Sn phase. The transition pressure for the ZB → RS was calculated to be 160 GPa for BP and 110 GPa for BAs. Full potential linearized augmented plane-wave (FP-LAPW) calculations showed that the ZB/RS coexistence pressure was 111 GPa in BP and 93 GPa in BAs [4].

Only a few theoretical works have been voted to the study of structural and electronic properties of BP and BAs. Recently, FP-LAPW calculations showed that the ZB phase of BP and BAs are indirect gap semiconductors [5,6]. Zaoui and co-worker carried out probably the most detailed and careful study of the electric and chemical bonding of these two compounds in the ZB phase at normal pressure [4]. The structural properties of BP have been determined by Lambrecht and Segall [7] using the linear muffin-tin orbitals (LMTO) method within the local density approximation (LDA). A comparative study of the structural and electronic properties of BP and BAs has been presented by Bouhaf et al. [8,9] using the plane-wave basis sets and pseudopotential approximation (PWPP) within LDA. However, these studies have been focused on the ZB phase of BP and BAs, and there have been few theoretical works on the electronic properties for the RS phase. FP-LAPW calculations showed that the RS phase of BP and BAs are metallic at the transition pressure [4]. However, Wentzcovitch and Cohen reported that the RS phase of BP is semimetal and BAs is metallic [3].

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In addition, several critical issues regarding the pressure-induced ZB to RS phase transition in these two compounds solid remain controversial. In this work, we performed first-principles calculations to investigate the phase transition of BP and BAs solid under high-pressure. Such study is not only important to address the controversies in the ZB → RS transition of these two compounds but also valuable for understanding the high-pressure behavior of the other III–V phosphide and arsenide compounds.

The rest of this paper is organized as follows: Section 2 gives the method of calculation. Results and discussion are given in Section 3 and finally in Section 4 the results are summarized and conclusions are drawn.

2. Computational details

Density functional calculations are conducted with the plane-wave pseudopotential method [10]. For these two compounds, the electronic exchange-correlation interactions are treated by the generalized gradient approximation (GGA) within the scheme due to Perdew–Burke–Ernzerhof (PBE) [11]. The norm-conserving pseudopotentials are employed to model the ion-electron interactions [12]. The energy cutoff of the plane-wave basis is chosen as 550 eV for BP and 440 eV for BAs. The Brillouin zone for the ZB and RS structures is sampled by the same Monkhorst–Pack [13] *k* points grids of 10 × 10 × 10 for BP and 9 × 9 × 9 for BAs, respectively. The chosen plane-wave cutoff and the number of k points were carefully checked to ensure the total energy converged to better than 1 meV/atom. For a given external hydrostatic pressure, both the parameters of the unit cell and the internal coordinates of the atoms are fully relaxed until forces had converged to less than 0.01 eV/Å. The relative stability of different structural phases is examined by comparing their enthalpy values, which are computed from $H = E + PV$.

3. Results and discussion

3.1. High-pressure structural transformations

The calculated equilibrium lattice parameters, zero-pressure bulk modulus(B), and its pressure derivative B' fitted from the third-order Birch–Murnaghan EOS [14] of BP and BAs for RS and ZB phases are summarized in Table 1, together with previous experiments [15,16] and other calculated results. We can see that, for the ZB phase, the calculated lattice constants are in good agreement with the experimental value with the errors less than 0.9% and 0.86%, respectively. We see, from this table, that our calculated values are in better agreement with the experimental and other theoretical calculation results, although there are no experimental reports for the RS structure.

Table 1
Structure parameters of BP and BAs in the zinc-blende and rocksalt structure calculated in equilibrium parameter and compared with theoretical and experimental data

Compound	Zinc-blende			Rocksalt	
	Present	Theoretical	Experimental	Present	Theoretical
BP					
a(Å)	4.495	4.53[1], 4.546[4], 4.498[5] 4.555[5], 4.51[7], 4.558[3,17]	4.538[15]	4.282	4.320[4]
B(GPa)	169	152[1], 166[3], 170[4] 176[5], 162[5], 172[7], 165[17]	173[16]	157	155[3], 171[4]
B'	3.61	4.3[1], 3.07[4] 3.92[5], 3.86[5], 3.7[7]		3.72	3.07[4]
BAs					
a(Å)	4.736	4.777[3], 4.784[4]4.741[6], 4. 817[6]	4.777[15]	4.546	4.583[3], 4.619[4]
B(GPa)	145	145[3], 137[4]147.5[6], 131. 2[6], 138[21]		147	143[3], 135[4]
B'	3.78	3.49[4], 4.216[6], 4. 179[6]		3.73	3.44[4]

In order to study the structural phase stability for BP and BAs, we applied hydrostatic pressure to these compounds with the ZB and RS phases up to 200 GPa and fully optimized both the lattice constants and the atomic positions. The computed relative enthalpy versus pressure curves in both the phases for these compounds are shown in Figs. 1 and 2, the calculated P–V relations of these two compounds are shown in Figs. 3 and 4. The transition pressure (p_t) is the pressure at which $H(P)$ curves for both phases crosses. In the case of BP, we can see from Figs. 1 and 3, the calculated value of p_t is 142 GPa, and the volume collapse is around 0.8%. Previous LDA calculations predicted the transformation pressure is found to be 160 GPa and accompanied with 8% volume reduction [3]. FP-LAPW calculations predicted the p_t of 111 GPa [4]. As we can see from

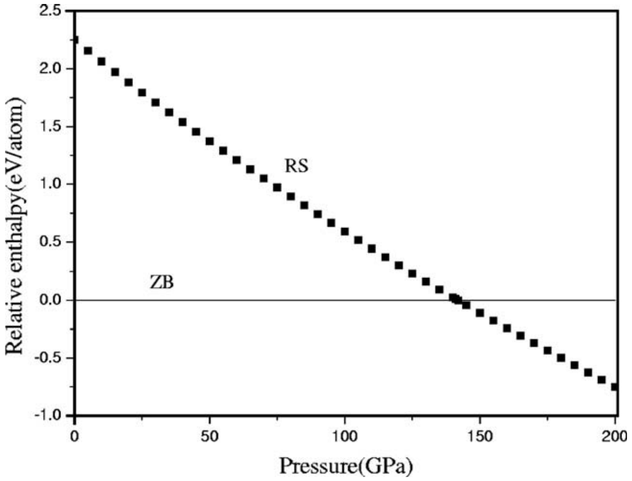

Fig. 1. Calculated enthalpy differences of the structure of BP with respect to the ZB structure as a function of pressure.

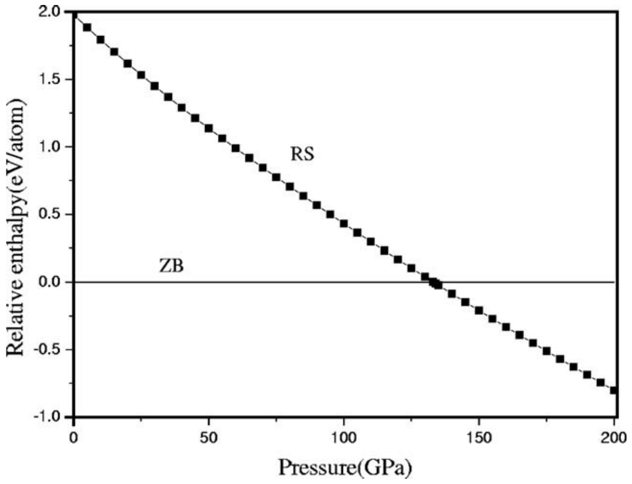

Fig. 2. Calculated enthalpy of ZB and RS phases of BAs as a function of pressure. The ZB phase has been taken as a reference.

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