Calculated electronic, transport, and related properties of zinc blende boron arsenide (zb-BAs)

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I. INTRODUCTION

Boron compounds have attracted great interests recently due to their important, technological applications, including those at high temperatures and in electronic and optical devices in the short wavelength range of the visible spectrum.1 These compounds possess unique physical properties such as exceedingly high thermal conductivity,2,3 as found in boron arsenide (BAs). Other properties include low dielectric, low densities,1 and large resistivities.4 Among Boron compounds, BAs is of particular interest not only because of its exceptionally high thermal conductivity but also for being the most covalent one. From the Van Vechten and Phillips scale of ionicity,5 boron is said to be more electronegative than arsenide. Some theoretical studies4,6 suggested that BAs shows the feature of inverse roles between the cation and anion. These studies explained that B plays the role of anion in BAs. This unusual behavior is attributed to the absence of p electrons in the core of the B atom and its small size.7 In a recent experimental work8 by Wang Shijun and his group, BAs was used as a p-type electrode and described as a suitable candidate for the photo-electrochemical and photovoltaic applications.

BAs remains relatively unexplored experimentally because of the difficulties in synthesizing a pure single crystal.5 It crystallizes in the zinc blende structure with a room temperature lattice constant of 4.777 Å.9 Cubic BAs is stable in the presence of arsenic vapor up to 920 °C; afterwards, it transforms into the rhombohedral structure.

Owing to the importance of BAs in various areas of technological applications,1 it has attracted a substantial number of theoretical calculations, ranging from several ab-initio local density approximations (LDA) and generalized gradient approximation (GGA) studies. We also found one GW calculation as well.

Ku10 estimated the experimental band gap of cubic BAs to be 1.46 eV. We could not determine from the article, however, whether or not the gap is direct. A recent work of Wang and his group11 reported an indirect, experimental band gap of 1.46 ± 0.02 eV for zb-BAs. They prepared a p-type boron arsenide photoelectrode, from a material consisting of a thin layer of boron arsenide on a boron substrate, in order to measure the gap given above. While these experimental values apparently agree with each other, the theoretical works discussed below are far from agreeing one with the others, or with experiment, for the band gap of zb-BAs. The relative emphasis on the band gap stems from its critical importance for the correct description of materials: when it is incorrect, the calculations cannot produce accurate optical transition energies, dielectric functions or densities of states (DOS) in agreement with the experiment.

Meradji et al.12 performed the relativistic, full potential, linearized augmented plane wave (FP-LAPW) calculations of the band gap of zb-Bas, using an LDA potential and obtained an indirect band gap of 1.13 eV. The LDA calculation of Anua and his group13 resulted in an indirect band gap of 1.12 eV. The FP-LAPW calculations of Wentzcovitch and Cohen,14 using the WIEN2k code and an LDA potential, led to an indirect band gap of 1.176 eV. When Anua and his...
group used an LDA, and a modified Becke and Johnson (mBJ) potentials, their indirect band gap was 1.730 eV. Wentzcovitch and Cohen\textsuperscript{15} employed the pseudopotential method to calculate the band gap of zb-BAs and obtained an indirect band gap value of 1.25 eV, using an LDA potential.

Ahmed and his group\textsuperscript{11} used FP-LAPW and the generalized gradient approximation (GGA) potentials to calculate the band gap of zb-BAs. They found an indirect band gap of 1.18 eV. When Ahmed \textit{et al}.\textsuperscript{11} used the GGA potentials of Engel and Vosko (GGA-EV), their value was 1.79 eV. Zaoui et al\textsuperscript{12} also used FP-LAPW and a GGA potential in their study of the electronic structure of zb-BAs and found an indirect band gap value of 1.23 eV. Meradji \textit{et al}.\textsuperscript{12} employed the augmented plane wave plus local orbital and a GGA potential to obtain an indirect band gap of 1.21 eV. Wentzcovitch and his co-workers\textsuperscript{15} also found a band gap of 1.25 eV using GGA potentials. Anua and his group\textsuperscript{13} used the FP-LAPW (WIEN2k) method with the GGA potential of Perdew, Burke, and Ernzerhof (PBE) and calculated a band gap of 1.235 eV. Their indirect band gap value was 1.142 eV, when they utilized the GGA potential of Wu and Cohen (GGA-WC). The first principle pseudopotential GGA calculations of Cui \textit{et al}.\textsuperscript{1} led to an indirect band gap of 1.32 eV. The 1989 pseudopotential calculations of Pickett,\textsuperscript{16} using GGA potentials, resulted in an indirect band gap of 1.23 eV. The norm-conserving pseudopotentials method of Boudjemline \textit{et al}.\textsuperscript{7} with a GGA potential, yielded an indirect band gap of 1.34 eV. Suth and his group\textsuperscript{17} reported the band gap values of 1.1 and 1.60 eV for their LDA and GW calculations, respectively. A first principle, self-consistent, orthogonalized-plane wave calculation (SCOPW) of Skutel\textsuperscript{9} yielded an indirect band gap of 1.6 eV from $\Gamma$ to X. Table I below provides a summary of these calculations for the band gap.

The above referenced \textit{ab-initio} LDA and GGA results, for the band gap of zb-BAs, mostly underestimate the experimental value of 1.46 eV. The modified Becke and Johnson potential led to an overestimate, i.e., 1.730 eV. While the results obtained with \textit{ab initio} LDA potentials vary from 1.1 eV to 1.176 eV, those from nine (9) GGA calculations range from 1.142 eV to 1.34 eV. The GGA potential of Engel and Vosko produced an overestimate, i.e., 1.79 eV. These discrepancies partly motivate our work. An added motivation stems from the potential applications of the material. Our work portends success in light of the fact that our method, the Bagayoko, Zhao, and Williams (BZW)\textsuperscript{18–22} as enhanced by Ekuma and Franklin (BZW-EF)\textsuperscript{23–28} using LDA and GGA potentials, has not only successfully described numerous semiconductors but also predicted the band gaps of cubic Si, cubic Na, cubic InN, and rutile TiO$_2$, which were later confirmed by the experiment.\textsuperscript{22} The rest of this paper is organized as follows: Section II describes the computational method. Section III presents our results. Discussions and the conclusion are given in Sections IV and V, respectively.

II. METHODS AND COMPUTATIONAL DETAILS

The computational method used in this work has been adequately described in the previous publications.\textsuperscript{22,23,25–27,29–33,36} We employed the local density approximation (LDA) potential of Ceperley and Alder,\textsuperscript{34} as parameterized by Vosko and his group\textsuperscript{35} and the linear combination of Gaussian orbitals (LCGO). The implementation of LCGO followed the Bagayoko, Zhao, and Williams (BZW)\textsuperscript{18,22,29–32} method, as enhanced by Ekuma and Franklin,\textsuperscript{22,25} in carrying out our self-consistent calculations. This method leads to the absolute minima of the occupied energies. Once these absolute minima of the occupied energies are attained, the method avoids unwarranted larger basis sets; such basis sets often cause some unphysical lowering of some unoccupied energies, including some of the lowest lying ones, without leading to any changes in the occupied ones.

Beginning with a small basis set, no smaller than the minimum basis set, the BZW-EF method\textsuperscript{23–27,36} requires successive and completely self-consistent calculations with the basis set being augmented in size and changing in angular and radial features. The minimum basis set is the one that is just large enough to account for all the electrons present in the material under study. The orbitals for the solid state

| Computational Methods | Potentials (DFT and others) | Eg (eV) |
|-----------------------|-----------------------------|--------|
| FP-LAPW LDA           | 1.13\textsuperscript{a}     |       |
| FP-LAPW LDA & WIEN2k  | 1.17\textsuperscript{c}     |       |
| FP-LAPW LDA & MBJ 1.79\textsuperscript{c} |       |
| Pseudopotential LDA   | 1.25\textsuperscript{g}     |       |
| Pseudopotential LDA   | 1.1\textsuperscript{e}      |       |
| FP-LAPW GGA           | 1.18\textsuperscript{b}     |       |
| FP-LAPW GGA-EV 1.79\textsuperscript{d} |       |
| FP-LAPW GGA           | 1.23\textsuperscript{b}     |       |
| Plane-wave (augmented) GGA | 1.21\textsuperscript{i}   |       |
| FP-LAPW GGA (PBE)     | 1.235\textsuperscript{c}    |       |
| FP-LAPW GGA (WU & Cohen) | 1.142\textsuperscript{d}   |       |
| Pseudopotential GGA   | 1.32\textsuperscript{b}     |       |
| Pseudopotential GGA   | 1.23\textsuperscript{b}     |       |
| Pseudopotential GGA   | 1.34\textsuperscript{f}     |       |
| Pseudopotential GW    | 1.60\textsuperscript{d}     |       |
| SCOPW 1.6\textsuperscript{e} |       |
| Experiment            | Vapor phase technique 1.46\textsuperscript{g} (type of gap not mentioned) |       |
|                       | 1.46 ± 0.02 (m) (indirect) \textsuperscript{h} |       |

\textsuperscript{a}Ref. 12.  
\textsuperscript{b}Ref. 13.  
\textsuperscript{c}Ref. 14.  
\textsuperscript{d}Ref. 15.  
\textsuperscript{e}Ref. 16.  
\textsuperscript{f}Ref. 4.  
\textsuperscript{g}Ref. 18.  
\textsuperscript{h}Ref. 9.  
\textsuperscript{i}Ref. 10.  
\textsuperscript{j}Ref. 8.  

The * implies that the computational, the potential, or the experimental methods were not clearly stated or not mentioned in the reference.
calculations are obtained from the self-consistent computations of electronic properties of the atoms or ions in the system. For zinc blende BAs, these species are B$^{+1}$ and As$^{-1}$. Except for the first one, each self-consistent calculation employs the basis set of the one preceding it, plus one orbital. In the original BZW, orbitals are added in the increasing order of the corresponding, excited state energies. The BZW-EF method recognizes the fact that polarization has supremacy over spherical symmetry in as much as the valence electrons, in multi-atomic materials, are concerned. Thus, in the BZW-EF method, orbitals are added in the order of the applicable $p$, $d$, or $f$ character, for a given principal quantum number ($n$), before the corresponding, spherical $s$ orbital.

The occupied energies of consecutive calculations are compared graphically, after setting the Fermi level to zero. Generally, many occupied energies from Calculation II are lower than corresponding ones from Calculation I. The lowering of some occupied energies in Calculation II signifies that the basis set of Calculation I was not complete in size, angular symmetry, and radial functions for the description of the ground state. Calculations III and IV and others follow Calculation II. The process of augmenting the basis set to perform a new calculation continues until the occupied energies from three ($3$) consecutive calculations N, (N + 1), and (N + 2) that are found to be the same, within our computational uncertainty of 5 meV. Among these calculations, N, the one with the smallest basis set, provides the density functional theory (DFT) description of the material. This choice is dictated by the fact that the Rayleigh theorem explains the artificial lowering of some unoccupied energies, by Calculation (N + 1) and the following ones, while these calculations do not change the charge density, the Hamiltonian, or an occupied energy. The basis set of Calculation N is called the optimal basis set; it is the smallest one required for the occupied energies to reach their absolute minima. With the BZW-EF method, the calculation directly following the optimal basis sets generally leads to the same low, unoccupied energies, as obtained with the optimal basis set, up to 10 eV. Basis sets much larger than the optimal one do not lower the occupied energies. The ones much larger than the optimal one continue to lower some unoccupied energies by virtue of the Rayleigh theorem.

We provide below the computational details needed for the replication of our work. We utilized a band structure program package developed at the Ames Laboratory of the Department of Energy, Ames, Iowa, for these calculations. The calculations are non-relativistic and are carried out at an experimental room temperature lattice constant of 4.777 Å.

We used the even-tempered Gaussian functions for the construction of atomic orbitals for boron and arsenide. The $s$ and $p$ orbitals were described using 16 even-tempered Gaussian functions for boron, with respective minimum and maximum exponents of 0.105 and 0.1365. For arsenide, the $s$ and $p$ orbitals were constructed using 24 even-tempered Gaussian functions, with the minimum and maximum exponents of 0.14 and 0.1499, respectively. Self-consistency was reached for the calculations after about 60 iterations. The iterations became sufficiently converged when the potentials from two consecutive ones are not different by more than 10$^{-5}$. The computational error made in accounting for the 26 valence electrons for BAs, after reaching self-consistency, is 0.00144 or 0.554 × 10$^{-4}$ per valence electron. We utilized a total of 81 k-points in the production of final, self-consistent band structure.

III. RESULTS

We present our results for energy bands, the total density of states (DOS), and the partial densities of states (pDOS), respectively, in Figures 1–3. The electronic band structure for zb-BAs, as shown in Figure 1, is from Calculations IV and V. According to the graphs of the bands and the numerical values of the eigenvalues, Calculations IV, V, and VI led to the same occupied energies, indicating that these energies have reached their absolute minima. It is also pertinent to note that Calculations IV and V also led to the same unoccupied energies up to +10 eV. According to the BZW-EF method, the fourth calculation is the one providing the DFT description of zb-BAs. Our calculated, indirect band gap of zb-BAs, from Γ-X, is 1.48 eV, which is in perfect agreement with the experimental value of 1.46 ± 0.02 eV. We calculated the direct band gap at Γ to be 3.30 eV, as shown in Table I. The minimum of the conduction band is between the Γ and X point, much closer to the latter.

The calculated energies at high symmetry points in the Brillouin zone are shown in Table III below. These energies are intended to ease comparisons with measured, optical transition energies and the future x-ray spectra of zb-BAs.

The total density of states (DOS) and partial densities of states (pDOS) are in Figures 2 and 3, respectively. These figures, along with Fig. 1 and Table II, provide the detailed description of the electronic energies of zb-BAs. From Fig. 2 and Table III, we see that the total width of the valence band is 15.172 eV and the width of the lowest valence band is 10.854 eV. We provide below the computational details needed for the replication of our work. We utilized a band structure program package developed at the Ames Laboratory of the Department of Energy, Ames, Iowa, for these calculations. The calculations are non-relativistic and are carried out at an experimental room temperature lattice constant of 4.777 Å.

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**FIG. 1.** The electronic band structure of zb-BAs, as obtained from Calculations IV (solid lines) and V (dashed lines), using an experimental lattice constant of 4.777 Å. The horizontal dotted line indicates the position of the Fermi energy (EF) which is set equal to zero. There is a perfect superimposition of the bands from calculations IV and V up to +10 eV. The calculated, indirect band gap is 1.48 eV from Γ to X.
The lowest laying peaks of the valence density of states are at \( I_C \) 12.07 and \( I_C \) 11.11 eV. The upper group of valence bands has a width of 8.753 eV and a prominent peak located at \( I_C \) 7.88 eV. Two other peaks are at \( I_C \) 5.70 eV and \( I_C \) 4.04 eV. The conduction band density of states exhibits a broad peak from 1.48 eV to beyond 8 eV, with two sharp spikes at 4.95 eV and 5.22 eV. It has a dip between the prominent peak and the other peaks. We see from Fig. 3 the different contributions of s, p, and d states. The lowest laying valence band is dominated by Arsenide 3s (As-3s), with very insignificant contributions from boron 2s (B-2s). The upper group of valence bands is mainly dominated by As-3p, B-2p, and B-2s, with tiny contributions from the As-3d. The conduction bands are mainly from a hybridization of As 3d and 3p states, with contributions from the B 2s and 2p states.

Effective masses are used in determining the transport properties of a system. Close to the minimum of the lowest conduction band at \( X \), the calculated electron effective masses in the units of \( m_0 \), along the \( X-U \) (longitudinal), \( X-U \) (transverse), \( X-W \) (transverse) directions, are 1.105, 0.232, and 0.232 \( m_0 \), respectively. The calculated, light hole effective masses in \( U-L \), \( U-X \), and \( U-K \) directions are 0.100, 0.120, and 0.135 \( m_0 \), respectively, and their average is 0.107 \( m_0 \). Our calculated, first heavy hole effective masses at the top of the valence band are as follows: \( M_{hh1} (\Gamma-U) \) [111] = 0.5 \( m_0 \), \( M_{hh1} (\Gamma-X) \) [100] = 0.239 \( m_0 \), and \( M_{hh1} (\Gamma-K) \) [110] = 0.448 \( m_0 \) (hh1-heavy hole one). In the same direction as the first, we calculated the second set of heavy hole effective masses with values as follows: \( M_{hh2} (\Gamma-U) \) [111] = 0.5 \( m_0 \), \( M_{hh2} (\Gamma-X) \) [100] = 0.209 \( m_0 \), and \( M_{hh2} (\Gamma-K) \) [110] = 0.234 \( m_0 \) (hh2-heavy hole two). To the best of our knowledge, there are no reported experimental results on the effective masses of zb-BAs. Skutel obtained from his calculations for the top of the valence band at \( U \), \( M_{hh1} (\Gamma-U) \) = 0.71 (heavy hole) and 0.14 (light hole) for the (1,1,1) direction and \( M_{hh1} (\Gamma-U) \) = 0.31 (heavy hole) and 0.26 (light hole) for the (1,0,0) direction. He also obtained an effective mass of about 1.2 for the conduction band minimum in the parallel and (1,0,0) directions.

### Table II: Successive LDA BZW-EF calculations of the band structure of zb-BAs, using the room temperature lattice constant of 4.777 Å. Calculation IV led to the absolute minima of the occupied energies, thereby providing the DFT description of zb-BAs. The superscript zero indicates an empty orbital.

| No | Valence orbitals for B\(^{\text{3+}}\) | Valence orbitals for As\(^{\text{3+}}\) | Total number of valence functions | Gap (\( \Gamma \)) in eV | Band gap (\( \Gamma-X \)) in eV | Gap (\( \Gamma-L \)) in eV |
|----|---------------------------------|---------------------------------|-------------------------------|-------------------|-------------------|-------------------|
| I  | \( 2s^2 \) \( 2p^0 \) | \( 3s^2 \) \( 3p^6 \) \( 3d^{10} \) \( 4s^2 \) \( 4p^4 \) | 34 | 3.873 | 3.055 | 3.995 |
| II | \( 2s^2 \) \( 2p^9 \) \( 3p^0 \) | \( 3s^2 \) \( 3p^6 \) \( 3d^{10} \) \( 4s^2 \) \( 4p^4 \) | 40 | 3.664 | 2.366 | 3.682 |
| III| \( 2s^2 \) \( 2p^9 \) \( 3p^0 \) | \( 3s^2 \) \( 3p^6 \) \( 3d^{10} \) \( 4s^2 \) \( 4p^4 \) \( 4d^0 \) | 50 | 3.385 | 1.514 | 3.314 |
| IV | \( 2s^2 \) \( 2p^9 \) \( 3p^0 \) \( 3d^0 \) | \( 3s^2 \) \( 3p^6 \) \( 3d^{10} \) \( 4s^2 \) \( 4p^4 \) \( 4d^0 \) | 60 | 3.301 | 1.484 | 3.093 |
| V  | \( 2s^2 \) \( 2p^9 \) \( 3p^0 \) \( 3d^0 \) | \( 3s^2 \) \( 3p^6 \) \( 3d^{10} \) \( 4s^2 \) \( 4p^4 \) \( 4d^0 \) | 64 | 3.292 | 1.465 | 3.041 |
| VI | \( 2s^2 \) \( 2p^9 \) \( 3p^0 \) \( 3d^0 \) \( 5s^0 \) | \( 3s^2 \) \( 3p^6 \) \( 3d^{10} \) \( 4s^2 \) \( 4p^4 \) \( 4d^0 \) \( 5s^0 \) | 64 | 3.293 | 1.461 | 3.041 |
Adherence to the conditions of the validity of DFT, using from those from the previous DFT calculations due to our completely self-consistent calculations, using an LDA potential constant, and the bulk modulus.

Densities of states, effective masses, the low-temperature lattice constant.

Figure 4 shows the total energy of zb-BAs versus the lattice constant. The minimum is at a lattice constant of 4.722 Å, 1.15% smaller than the room temperature value. The band gap at zero temperature is 1.451 eV and is indirect. Our calculated bulk modulus is 138.62 GPa.

IV. DISCUSSIONS

Our rigorous implementation of the BZW-EF method guaranteed that our results have the full, physical content of DFT (or LDA). The attainment of the absolute minima of the occupied energies and the avoidance of over-complete basis sets led to our adherence to the conditions of the validity of DFT and of LDA, using the BZW-EF method. Unlike the many previous, calculated band gaps in Table 1, our findings agree perfectly with experiment. The presumed utilization of a single basis set approach in these previous works means that their outcomes do not necessarily possess the physical content of DFT. Hence, their deviations from experiment should be expected.

V. CONCLUSION

We have described the ground state electronic, transport, and related properties of zb-BAs with ab-initio and completely self-consistent calculations, using an LDA potential and the LCGO formalism. Our calculation results differ from those from the previous DFT calculations due to our adherence to the conditions of the validity of DFT, using the BZW-EF method. Our calculated band gap of 1.48 eV is in excellent agreement with experiment. The future experimental results are expected to confirm our findings for the densities of states, effective masses, the low temperature lattice constant, and the bulk modulus.

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FIG. 4. The total energy per electron (in eV) of BAs versus the lattice constant.
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