LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Electronic Properties of Aluminum Phosphide (AlP)

Azizjon Saliev

Department of Electrical and Computer Engineering, Binghamton University, New York

Department of Physics, Southern University and A&M College, Baton Rouge, Louisiana

Abstract

- In this presentation, we will discuss results of our calculations on electronic properties of zinc blende aluminum phosphide (AlP).

- We performed *ab-initio,* self-consistent calculations using local density functional potential, following Bagayoko, Zhao, and Williams method as enhanced by Ekuma, Franklin (BZW-EF).

- We also employed Local Density Approximation (LDA) and Linear Combination of Atomic Orbitals (LCAO).

Outline

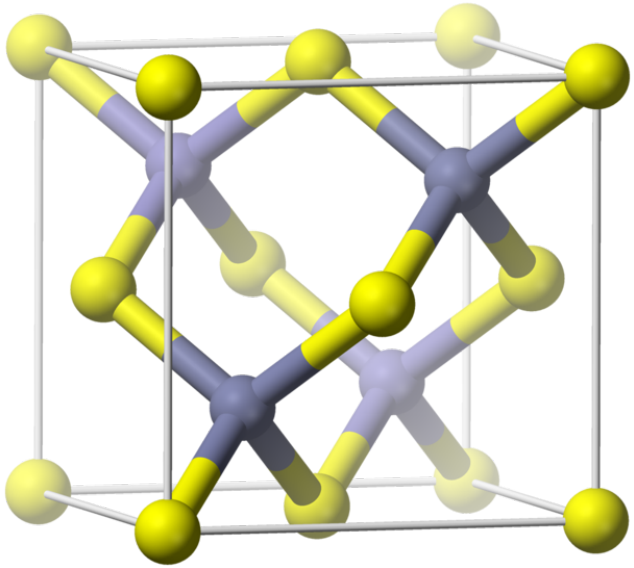
- Introduction
- Methodology
- Calculation & Results
- Discussion
- Conclusion
- Acknowledgment and References

Introduction

- Why AlP is so important to study?
- *AlP is a wide gap III-V group semiconductor material*
- *AlP is used in semiconductor industry for the fabrication of microelectronic devices*
- *due to its fumigant property, it is widely used in agricultural fields across the world*

Introduction:

Some properties of AlP



-- AlP is an *indirect* wide gap semiconductor

-- The minimum of the conduction bands is located at the X point of the Brillouin zone

--The top of the valence band is at the Gamma point.

Motivation for this work

- Previous *ab-initio* LDA and GGA calculations found band gaps of 1.46, 1.47, 1.54, and 1.64 eV – 30% or more smaller than the experimental one.

- Experimental measurements agree on a room a low temperature indirect band gaps of 2.43 ± 0.2 eV and 2.50-2.52 eV, respectively.

- The totally unsatisfactory theoretical findings motivated this work.

Methodology

- In our computation we employed Ceperley and Alder's LDA and linear combination of atomic orbitals (LCAO).

- We utilized the BZW-EF method in the implementation of the LCAO: Successive calculations, with increasing sizes of the basis sets, were performed **until the occupied energies reached their absolute minima.**

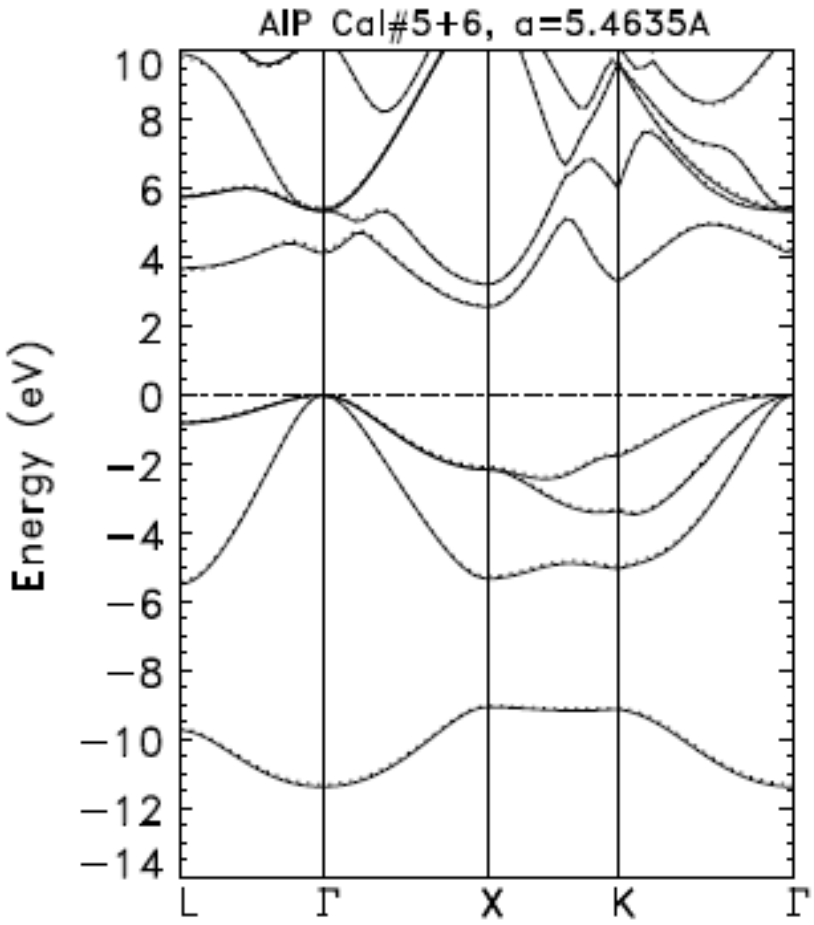
- In the methodical increase of the basis sets, p, d, and f orbitals are added before the spherically symmetric s orbital for the same principal quantum number (primacy of polarization over spherical symmetry for valence electron in molecules and solids)

Calculation and Results

- Calculation I: occupied energy orbitals only - minimum basis (MB) set
- Next calculations: orbitals were added as shown in the table below. s
- For all *ab-initio,* self-consistent calculations: l.c. a 5.4635 Å, *T* = 300K

	Aluminum (Al) (valence electrons)	**Phosphorus (P) (valence electrons)**	**No. of States (Orbs)**	**BG in eV (Γ- X)**
Calc I	$2s^2 2p^6 3s^2 3p^1$	$2s^2 2p^6 3s^2 3p^3$	8+8=16*2=32	**4.185**
Calc II	$2s^2 2p^6 3s^2 3p^1 3d^0$	$2s^2 2p^6 3s^2 3p^3$	13+8=21*2=42	**2.891**
Calc III	$2s^2 2p^6 3s^2 3p^1 3d^0$	$2s^2 2p^6 3s^2 3p^3 3d^0$	13+13=26*2=52	**2.890**
Calc IV	$2s^2 2p^6 3s^2 3p^1 3d^0 4p^0$	$2s^2 2p^6 3s^2 3p^3 3d^0$	16+13=29*2=58	**2.662**
Calc V	**$2s^2 2p^6 3s^2 3p^1 3d^0 4p^0$**	**$2s^2 2p^6 3s^2 3p^3 3d^0 4p^0$**	**16+16=32*2=64**	**2.561**
Calc VI	$2s^2 2p^6 3s^2 3p^1 3d^0 4p^0 4d^0$	$2s^2 2p^6 3s^2 3p^3 3d^0 4p^0$	21+16=37*2=74	**2.603**

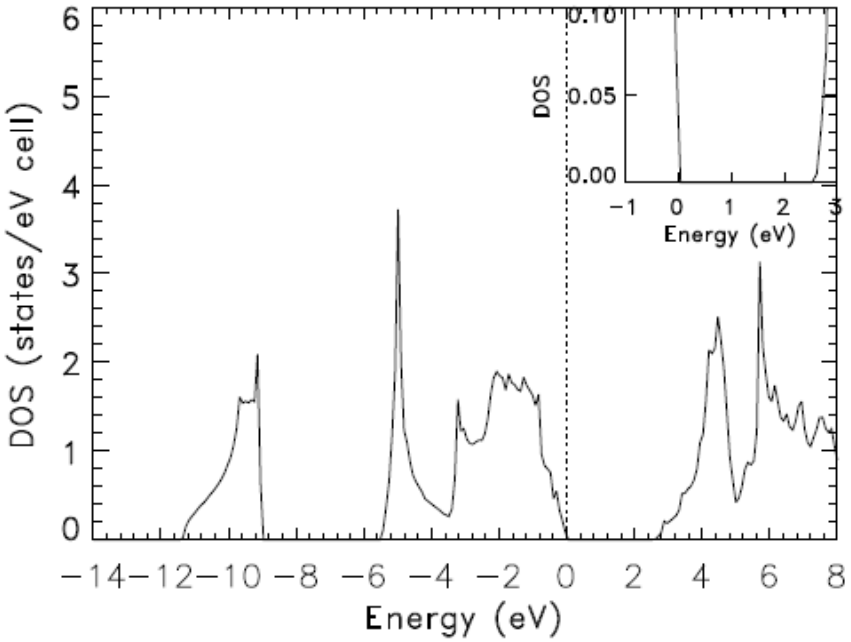
Calculation and Results



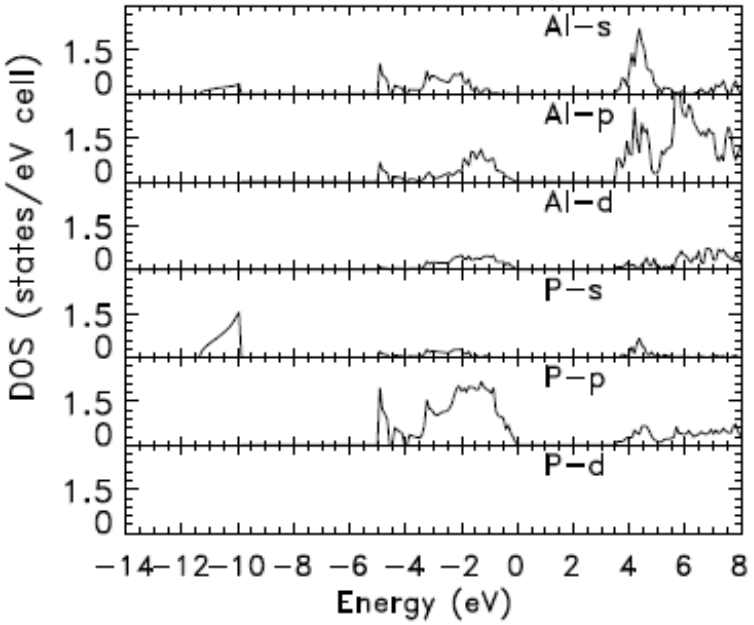
- Comparison of Calculations I and V:I resulted in Calculation V to be chosen as *optimal set.*
- Calculated, indirect band gap (Γ-X) of 2.56 eV
- Excellent agreement with the experimental band gap of 2.43 +- 0.2 eV

Densities of States

Total Density of States



Partial Density of States



Effective Masses

At the valence band maximum, we obtained the following heavy-hole masses:

$m_{\Gamma\text{-}l}$ = 1.301 m_0, $m_{\Gamma\text{-}x}$ = 0.544 m_0, and two heavy-hole masses at K point - $m_{\Gamma\text{-}k}$ = 0.615 m_0 and $m_{\Gamma\text{-}k}$ = 0.500 m_0.

Light-hole masses are $m_{\Gamma\text{-}l}$ = 0.177 m_0, $m_{\Gamma\text{-}x}$ = 0.253 m_0, and $m_{\Gamma\text{-}l}$ = 0.219 m_0.

The calculated electron effective masses, at the minimum of the conduction band, are 0.793 (X-Γ), 0.898 (X-K), and 0.305 (X-W).

Discussion

Previous *ab-initio* LDA and GGA calculations led to band gaps much smaller than the experimental ones.

The excellent agreement between our result and the corresponding experimental one is due to our use of the BZW-EF method.

Indeed, the method meets the variational requirements imposed by the derivation of DFT.

Conclusion

- We performed *ab-initio,* self-consistent calculations of the electronic energy bands, the total (DOS) and partial (pDOS) densities of states, and of electronic and hole effective masses of zinc blende aluminum phosphide (zb-AlP).

- In our calculations, we employed an LDA potential, the LCAO formalism, and the Bagayoko, Zhao, and Williams method as enhanced by Ekuma and Franklin (BZW-EF). We used the room temperature lattice constant.

- Our calculations yielded a band gap of 2.56 eV which is in excellent agreement with the experimental data of 2.43 ± 0.2 eV, at room temperature.

Acknowledgment and References

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