Electronic Properties of Aluminum Phosphide (AIP)

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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 \textit{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 $2.43 \pm 0.2$ 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.
- For all **ab-initio**, self-consistent calculations: l.c. a 5.4635 Å, $T = 300K$

<table>
<thead>
<tr>
<th></th>
<th>Aluminum (Al)</th>
<th>Phosphorus (P)</th>
<th>No. of States (Orbs)</th>
<th>BG in eV ($\Gamma$- X)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calc I</td>
<td>$2s^22p^6,3s^23p^1$</td>
<td>$2s^22p^6,3s^23p^3$</td>
<td>8+8=16*2=32</td>
<td>4.185</td>
</tr>
<tr>
<td>Calc II</td>
<td>$2s^22p^6,3s^23p^13d^0$</td>
<td>$2s^22p^6,3s^23p^3$</td>
<td>13+8=21*2=42</td>
<td>2.891</td>
</tr>
<tr>
<td>Calc III</td>
<td>$2s^22p^6,3s^23p^13d^0$</td>
<td>$2s^22p^6,3s^23p^33d^0$</td>
<td>13+13=26*2=52</td>
<td>2.890</td>
</tr>
<tr>
<td>Calc IV</td>
<td>$2s^22p^6,3s^23p^13d^04p^0$</td>
<td>$2s^22p^6,3s^23p^33d^0$</td>
<td>16+13=29*2=58</td>
<td>2.662</td>
</tr>
<tr>
<td>Calc V</td>
<td>$2s^22p^6,3s^23p^13d^04p^0$</td>
<td>$2s^22p^6,3s^23p^33d^04p^0$</td>
<td>16+16=32*2=64</td>
<td>2.561</td>
</tr>
<tr>
<td>Calc VI</td>
<td>$2s^22p^6,3s^23p^13d^04p^04d^0$</td>
<td>$2s^22p^6,3s^23p^33d^04p^0$</td>
<td>21+16=37*2=74</td>
<td>2.603</td>
</tr>
</tbody>
</table>
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:

\[ m_{\gamma-l} = 1.301 \, m_0, \quad m_{\gamma-x} = 0.544 \, m_0, \] and two heavy-hole masses at K point - \[ m_{\gamma-k} = 0.615 \, m_0 \] and \[ m_{\gamma-k} = 0.500 \, m_0. \]

Light-hole masses are \[ m_{\gamma-l} = 0.177 \, m_0, \quad m_{\gamma-x} = 0.253 \, m_0, \] and \[ m_{\gamma-l} = 0.219 \, m_0. \]

The calculated electron effective masses, at the minimum of the conduction band, are 0.793 (X-\( \Gamma \)), 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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