Band Structure Analysis of Diamond and Zinc-blende Semiconductors Using Pseudopotential Methods

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***Abstract*—This project presents a comprehensive computational analysis of electron band structures for fourteen semiconductors with diamond and zinc-blende crystal structures. Using pseudopotential form factors derived from Cohen and Bergstresser's work, the band structures were computed and analyzed. The work demonstrates the effectiveness of the Bloch model in reciprocal space calculations and provides insights into the electronic properties of these fundamental semiconductor materials.**

I. Introduction

The investigation of electron band structures in semiconductors is crucial for understanding their electronic properties and technological applications. This study focuses on fourteen semiconductors with face-centered cubic (FCC) crystal structures, including both diamond and zinc-blende types. These materials form the foundation of modern semiconductor technology.

The computation relies on the Bloch model, which introduces a periodic potential $V(\mathbf{r})$, independent of time:

$$V(\mathbf{r}) = V(\mathbf{r} + \mathbf{R}_n) \tag{1}$$

where $\mathbf{r}$ represents the position vector, and $\mathbf{R}_n$ denotes lattice vectors. This periodicity allows the potential to be expanded as a Fourier series:

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} \tag{2}$$

where $\mathbf{G}$ represents reciprocal lattice vectors, and $V_{\mathbf{G}}$ are the pseudopotential form factors. For FCC structures, the form factor is given by:

$$V_{\mathbf{G}} = \frac{V_S}{|\mathbf{G}|^2}\cos(\mathbf{G}\cdot\mathbf{s}) + i\frac{V_A}{|\mathbf{G}|^2}\sin(\mathbf{G}\cdot\mathbf{s}) \tag{3}$$

where $\mathbf{s} = \frac{a}{8}(1,1,1)$ and V_S and V_A are experimental fits from Cohen's work.

II. Methodology

The computational approach follows these key steps:

1) Definition of the Brillouin zone (BZ) path using the Monkhorst and Pack method
2) Application of cutoff to reciprocal lattice vectors: $V_{\mathbf{G}} = 0$ for $|\mathbf{G}|^2 > 11(4\pi^2/a^2)$
3) Construction of the Hamiltonian matrix in reciprocal space
4) Matrix diagonalization to obtain eigenvalues and eigenvectors

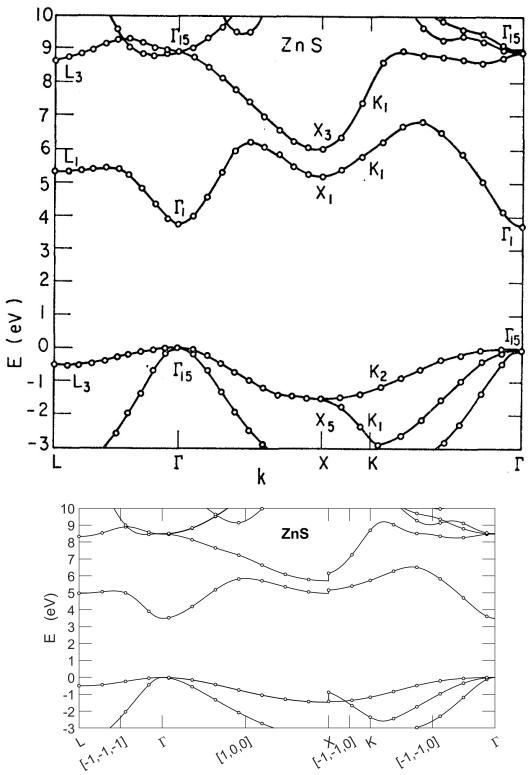
The Schrödinger equation in reciprocal space transforms into the matrix eigenvalue problem:

$$[H(\mathbf{k}) - IE]c(\mathbf{k}) = 0 \tag{4}$$

III. Results and Discussion

A. Silicon (Si)

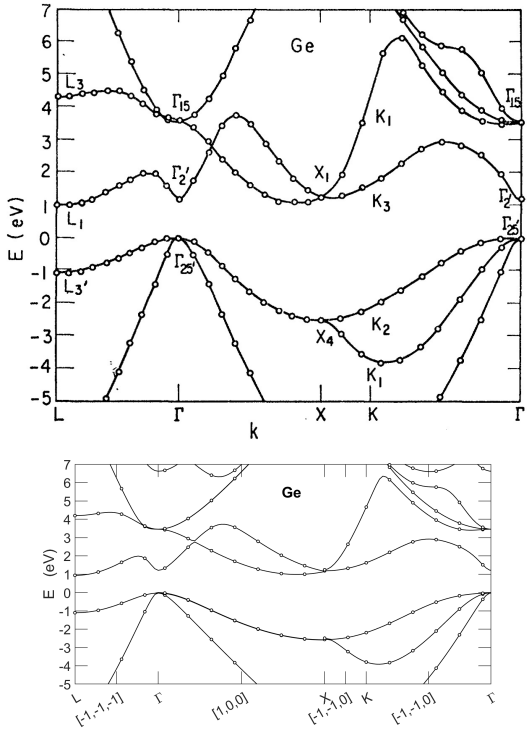
Silicon, as a cornerstone material in semiconductor technology, demonstrates the characteristic indirect band gap. The computed results closely match the reference data, validating the pseudopotential parameters used.



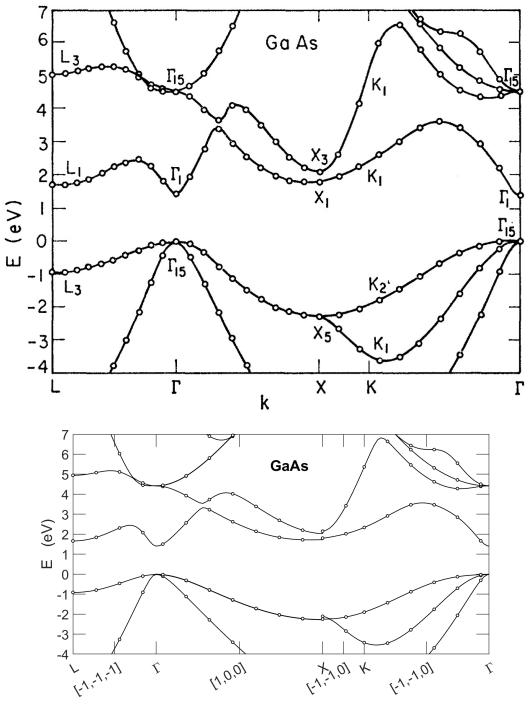
Silicon band structure comparison

B. Germanium (Ge)

Germanium's band structure highlights its narrow band gap and unique electronic properties. The simulation effectively captures its indirect gap and energy dispersion characteristics.



Germanium band structure comparison



Germanium band structure comparison

C. III-V Compounds

The band structures of III-V compounds (GaAs, GaP, AlSb, InP, GaSb, InAs, InSb) show distinct characteristics:

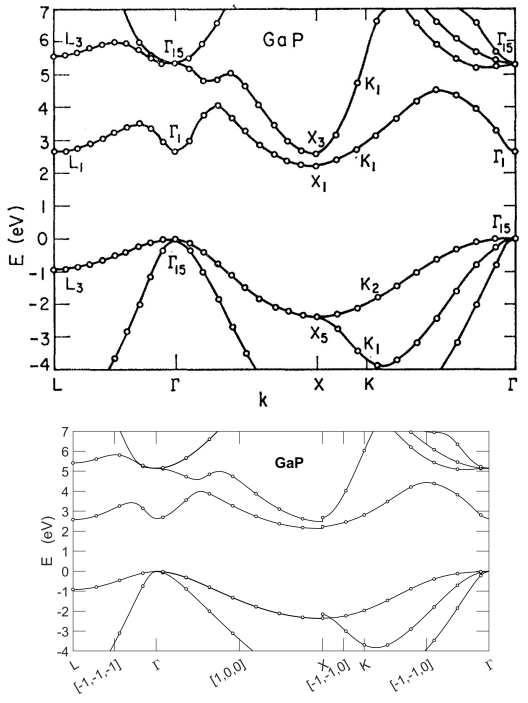
- GaAs exhibits its characteristic direct band gap at Γ.
- Split of X_1 into X_1 and X_3 for homopolar substances.
- $\Gamma_{2'}$ level shows decreasing energy for heavier semiconductors.
- L_1 demonstrates a downward trend relative to X_1 level.

D. II-VI Compounds

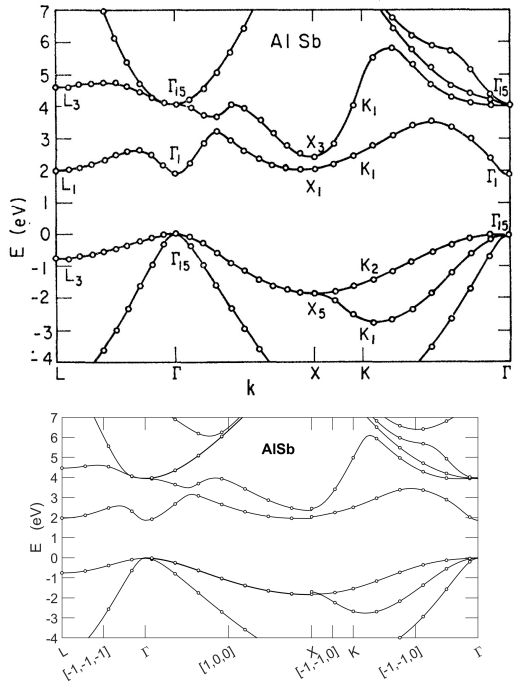
The zinc-blende structures (ZnS, ZnSe, ZnTe, CdTe) generally exhibit higher band gaps compared to diamond structures, demonstrating the importance of atomic composition in determining electronic properties.

IV. Conclusion

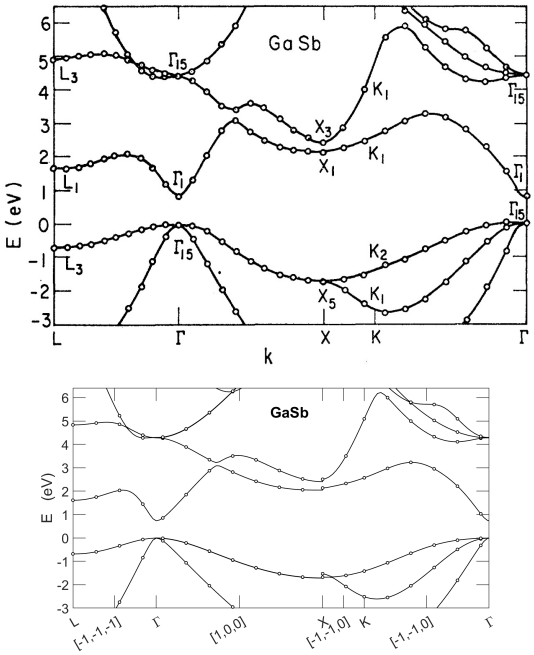
The computational analysis of fourteen semiconductors validates the effectiveness of pseudopotential methods in band structure calculations. The results show excellent agreement with reference data, particularly in reproducing key features such as band gaps, energy dispersions, and level splitting. The success in simulating these diverse materials reaffirms the validity of the Bloch model for FCC structured semiconductors.



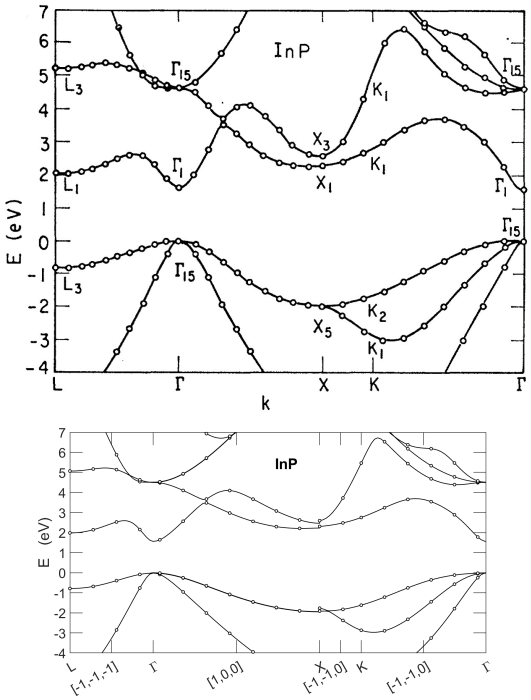
GaP band structure comparison



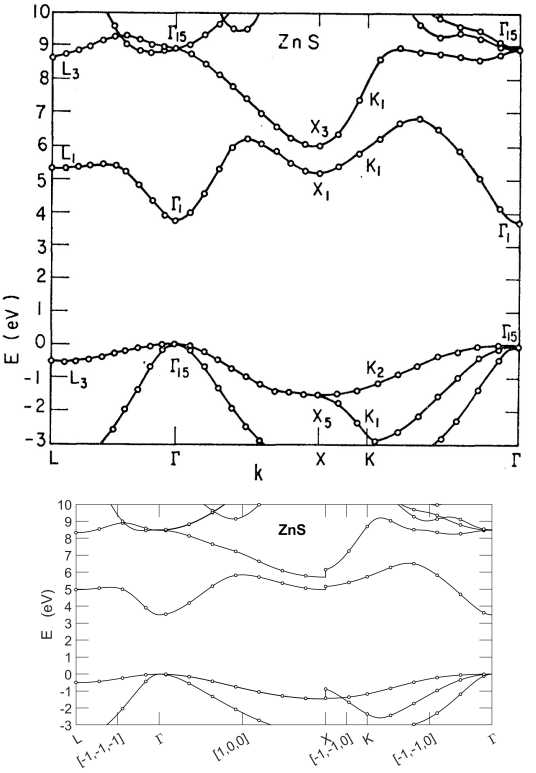
AlSb band structure comparison



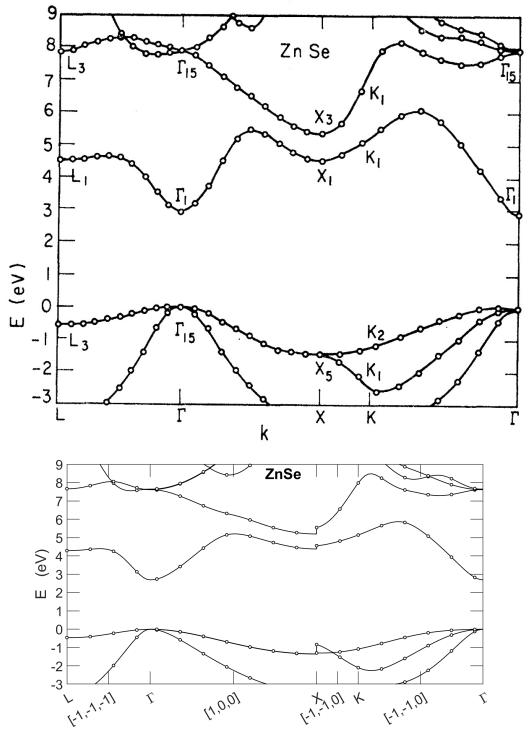
GaSb band structure comparison



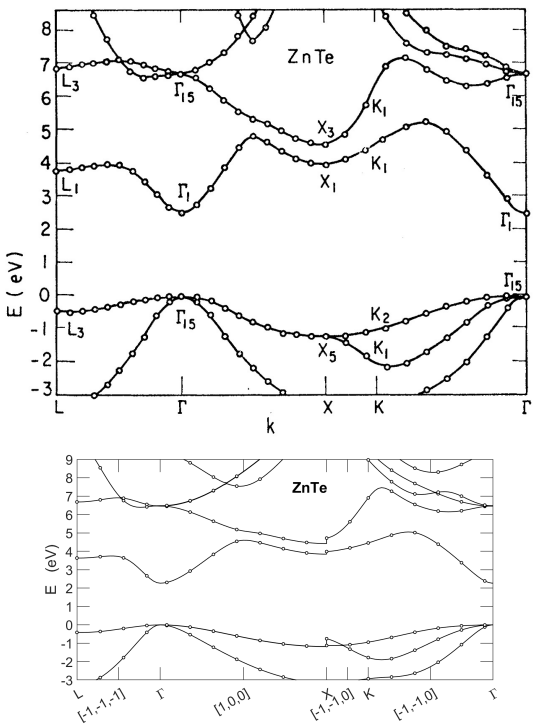
InP band structure comparison



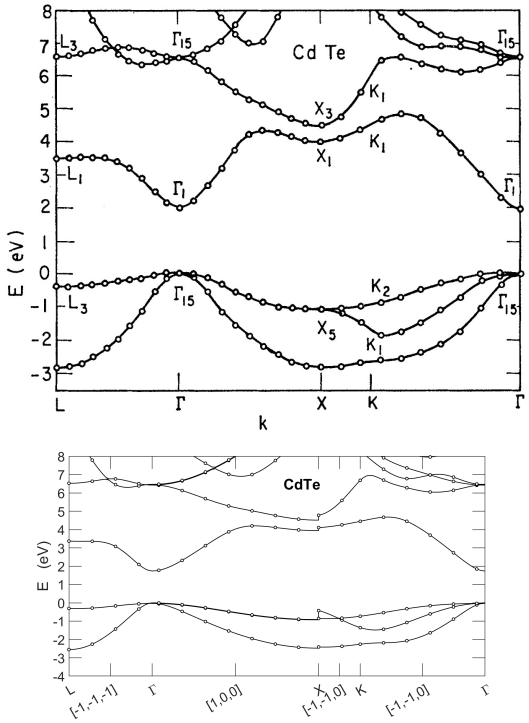
ZnS band structure comparison



ZnSe band structure comparison



ZnTe band structure comparison



CdTe band structure comparison

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[1] M. L. Cohen and T. K. Bergstresser, "Band structures and pseudopotential form factors for fourteen semiconductors of the diamond and zinc-blende structures," *Phys. Rev.*, vol. 141, pp. 789–796, 1966.

[2] H. J. Monkhorst and J. D. Pack, "Special points for brillouin-zone integrations," *Phys. Rev. B*, vol. 13, pp. 5188–5192, 1976.