Electron Band Structure Calculations for 14 Semiconductors

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***Abstract*—This study reproduces pseudopotential form factors and electron band structures for 14 semiconductors with diamond and zincblende structures. Examining materials - AlSb, CdTe, GaAs, GaP, GaSb, Ge, InAs, InP, InSb, Si, Sn, ZnS, ZuSe, and ZnTe, this paper meticulously aligns with experimental data and results closely mirror M.L. COHEN and T. K. BERGSTRESSER's original work (Physical Review 141, 789, 1966). This concise examination contributes to the validation and extension of the seminal band structures.**

I. Introduction

The objective of this study is to compute the electron band structure of 14 semiconductors listed in Table 3.2 of the lecture notes. The Brillouin zone path used in the calculations is defined by the function 'BZpath.m', as specified in Exercise 3.8.6 of the lecture notes. The correctness of the results will be validated against the paper by M.L. Cohen and T. K. Bergstresser, titled "Band Structures and Pseudopotential Form Factors for Fourteen Semiconductors of the Diamond and Zinc-blende Structures" (Physical Review 141, 789, 1966)[1]. The focus is on precision to experimental observations, with minimal discussion, mirroring the original approach. The subsequent sections detail the pseudopotential Hamiltonian, form factor determination, and present the reproduced results.

II. Theory

The Hamiltonian governing the electron's behaviour within the crystal comprises a kinetic energy component and a spatially dependent weak potential.

$$-(\hbar^2/2m)\nabla^2 + V(\mathbf{r}) \tag{1}$$

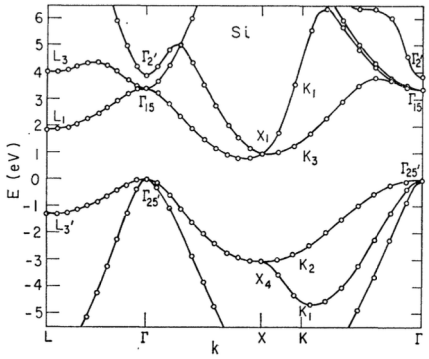
The potential V can be Fourier-expanded in reciprocal lattice vectors **G** and represented as the product of a structure factor **S(G)** and a pseudopotential form factor V_G. It is convenient to decompose the potential into symmetric and asymmetric components.

$$V(\mathbf{r}) = \sum_{|G|\leq G_0} (S^s(\mathbf{G})V_G^s + iS^A(\mathbf{G})V_G^A)e^{-iG\cdot\mathbf{r}} \tag{2}$$

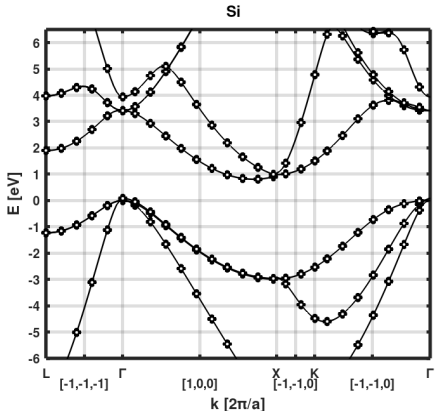
Further, the methodology employed in obtaining the electron band structures closely adheres to the procedures outlined in the original paper [1] and in the lecture notes of chapter 3 (sections 3.1 to 3.3) which follows the same set of equations. The same approach and techniques have been meticulously followed, ensuring consistency and reliability in the reproduction of the band structures for the 14 semiconductors.

III. Results

A rigorous comparison has been conducted between the replicated band structures and pseudopotential form factors, as presented in the following figures, and the original outcomes from Cohen and Bergstresser's seminal work (Physical Review 141, 789, 1966). The figures illustrate a compelling alignment between the reproduced results and the established findings, reinforcing the accuracy of the computational approach. This meticulous analysis affirms the consistency and reliability of the replicated electron band structures for the 14 semiconductors with diamond and zinc-blende structures. Figures 1 to 14 provide a comprehensive comparison between the electron band structures of various semiconductors, as reported in the original paper by Cohen and Bergstresser, and the reproduced results obtained in this study. Each figure corresponds to a specific semiconductor, as indicated in the respective caption, facilitating a clear visual inspection of the agreement between the original and reproduced band structures. Notably, the results exhibit a substantial and consistent match across all semiconductors, validating the accuracy of the reproduced band structures against the seminal work of Cohen and Bergstresser. This comparative analysis serves as a robust verification of the reliability of the computational approach employed in reproducing the electron band structures.

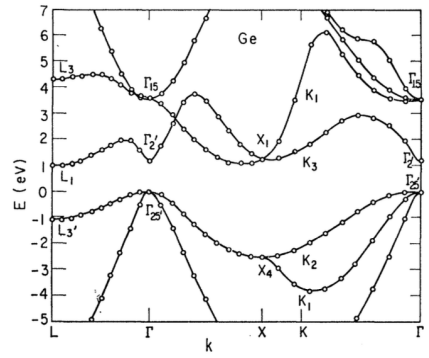


(a) Band Structure for Si as in the original paper

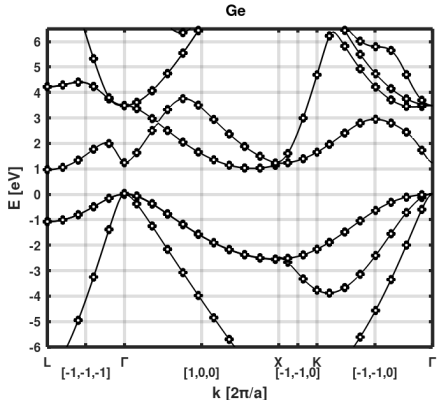


(b) Reproduced Band Structure for Si

Fig. 1: Comparison of Band Structures for Silicon

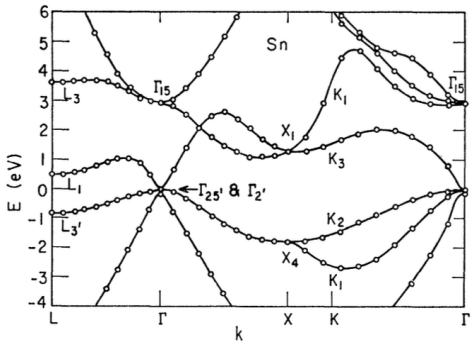


(a) Band Structure for Ge as in the original paper

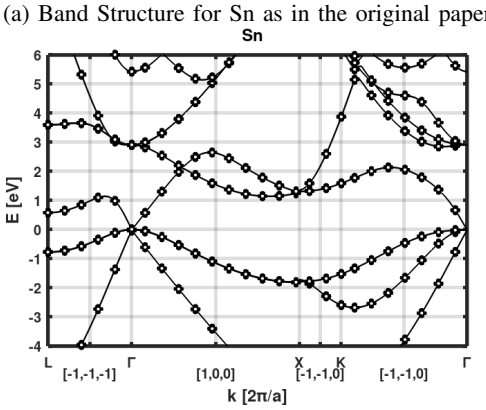


(b) Reproduced Band Structure for Ge

Fig. 2: Comparison of Band Structures for Ge

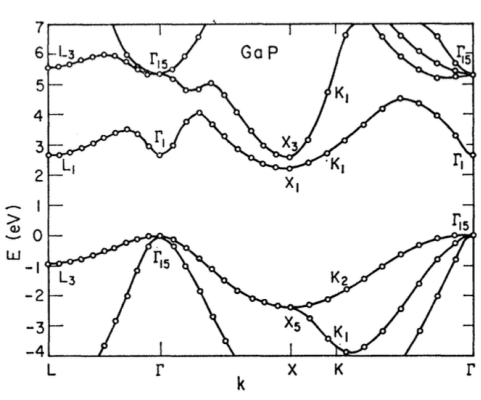


(a) Band Structure for Sn as in the original paper

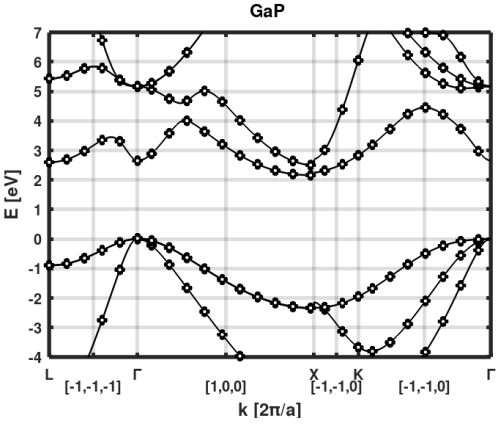


(b) Reproduced Band Structure for Sn

Fig. 3: Comparison of Band Structures for Sn

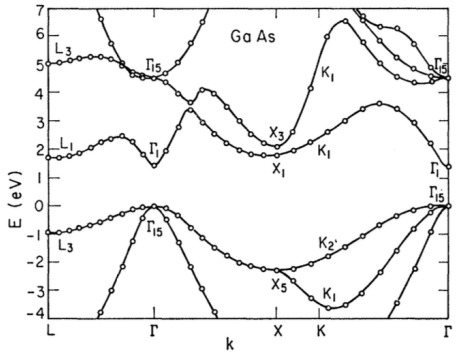


(a) Band Structure for GaP as in the original paper

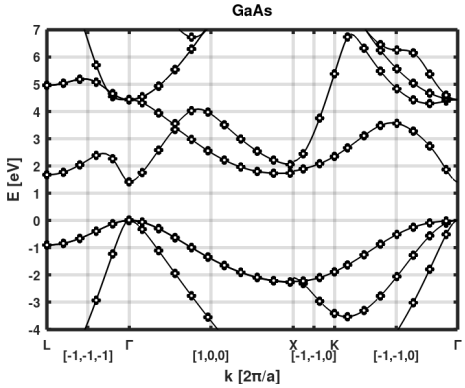


(b) Reproduced Band Structure for GaP

Fig. 4: Comparison of Band Structures for GaP

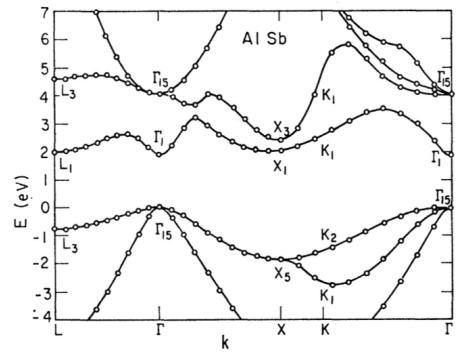


(a) Band Structure for GaAs as in the original paper

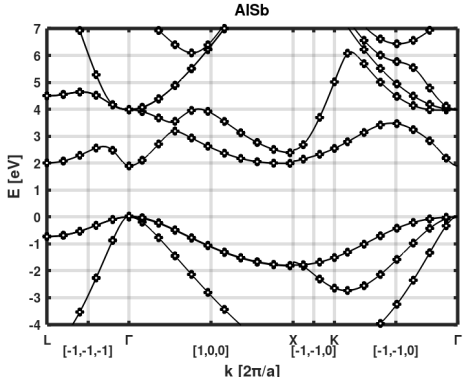


(b) Reproduced Band Structure for GaAs

Fig. 5: Comparison of Band Structures for GaAs

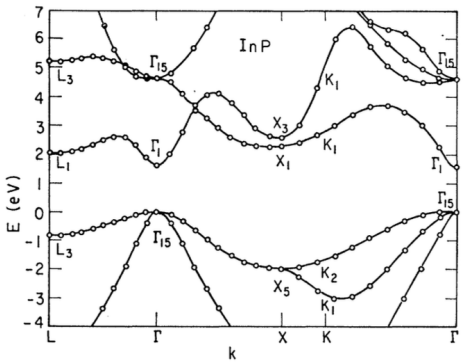


(a) Band Structure for AlSb as in the original paper

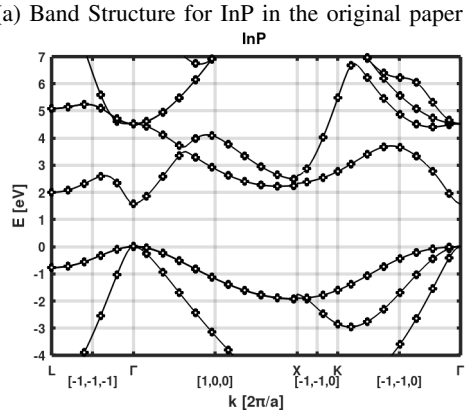


(b) Reproduced Band Structure for AlSb

Fig. 6: Comparison of Band Structures for AlSb

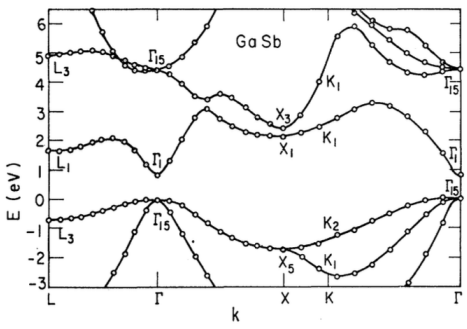


(a) Band Structure for InP in the original paper

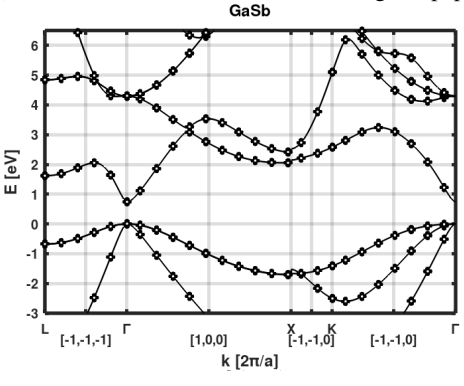


(b) Reproduced Band Structure for InP

Fig. 7: Comparison of Band Structures for InP

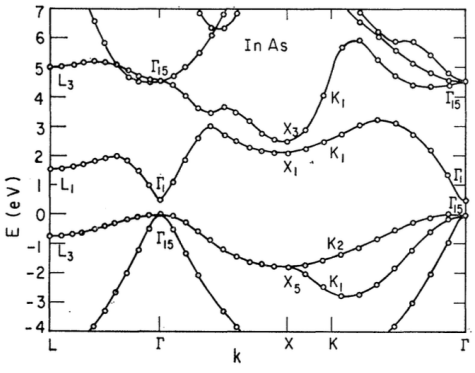


(a) Band Structure for GaSb in the original paper

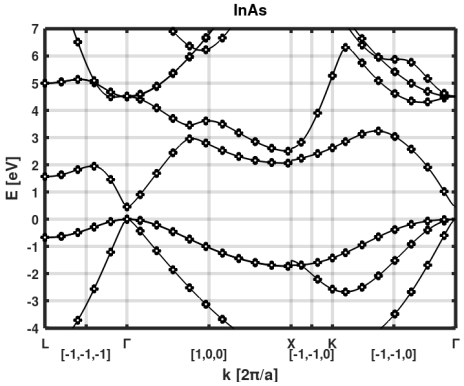


(b) Reproduced Band Structure for GaSb

Fig. 8: Comparison of Band Structures for GaSb

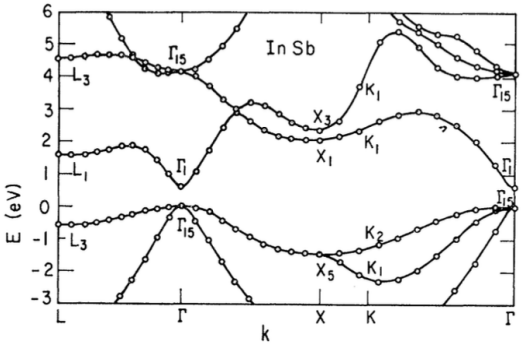


(a) Band Structure for InAs in the original paper

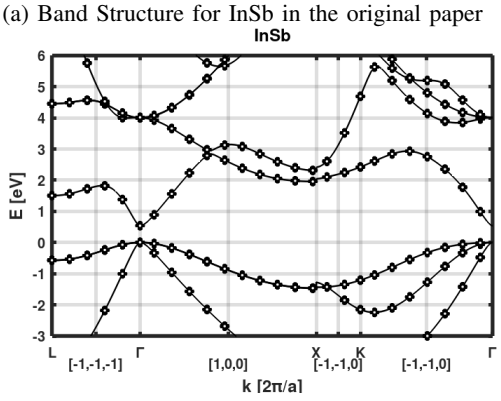


(b) Reproduced Band Structure for InAs

Fig. 9: Comparison of Band Structures for InAs

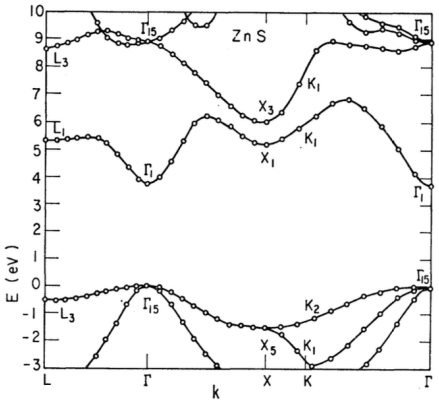


(a) Band Structure for InSb in the original paper

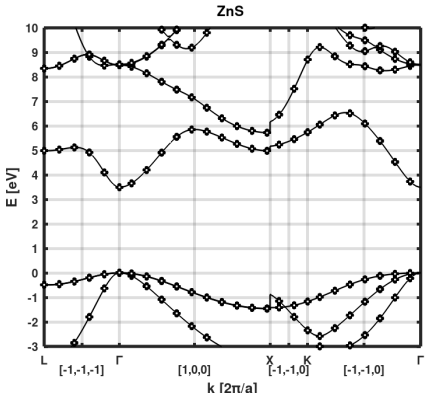


(b) Reproduced Band Structure for InSb

Fig. 10: Comparison of Band Structures for InSb

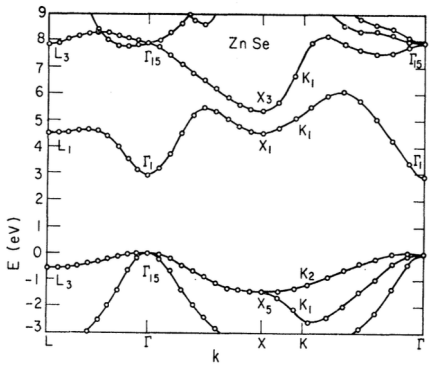


(a) Band Structure for ZnS in the original paper

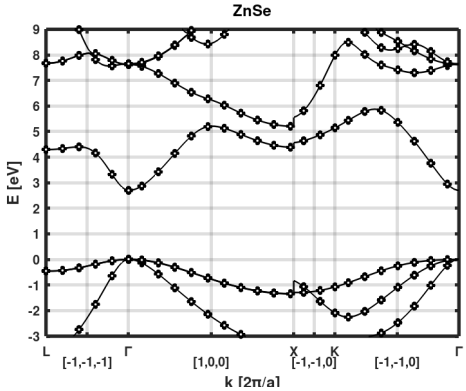


(b) Reproduced Band Structure for ZnS

Fig. 11: Comparison of Band Structures for ZnS

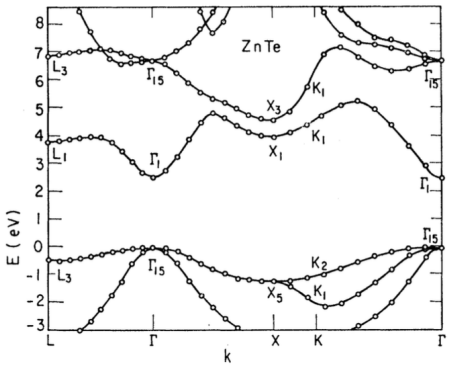


(a) Band Structure for ZnSe in the original paper

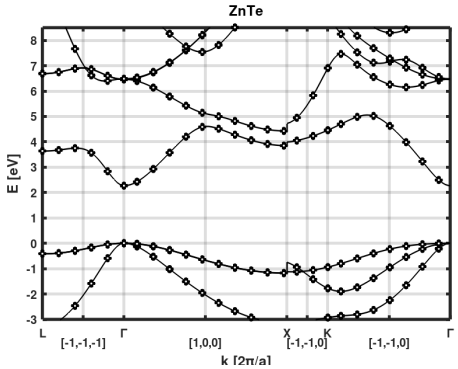


(b) Reproduced Band Structure for ZnSe

Fig. 12: Comparison of Band Structures for ZnSe

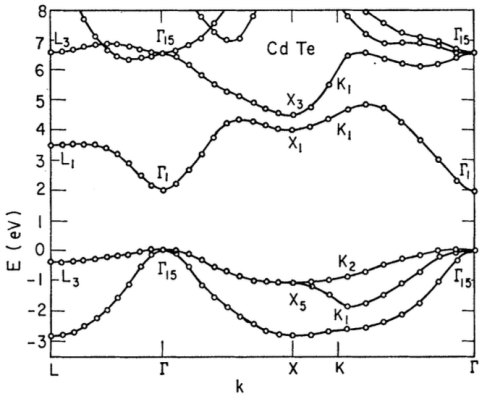


(a) Band Structure for ZnTe in the original paper

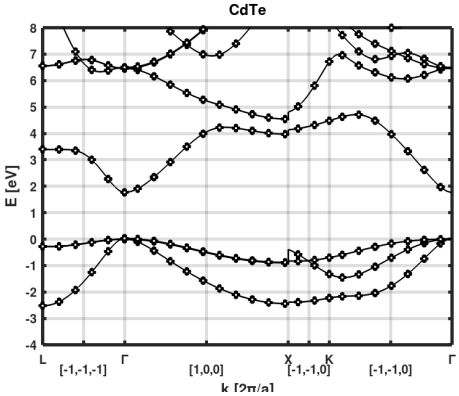


(b) Reproduced Band Structure for ZnTe

Fig. 13: Comparison of Band Structures for ZnTe



(a) Band Structure for CdTe in the original paper



(b) Reproduced Band Structure for CdTe

Fig. 14: Comparison of Band Structures for CdTe

IV. Conclusion

This study successfully reproduced the electron band structures of 14 semiconductors, validating Cohen and Bergstresser's work. The comprehensive comparison, depicted in Figures 1 to 14, demonstrates a consistent match across all materials. The accuracy of the replicated outcomes affirms the reliability of the computational approach and contributes to the understanding of electron behaviour in crystals.

References

[1] Marvin L Cohen and TK Bergstresser. Band structures and pseudopotential form factors for fourteen semiconductors of the diamond and zinc-blende structures. *Physical Review*, 141(2):789, 1966.