Solid State Physics Homework 2

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1 Introduction

The pseudopotential method is a computational approach in solid-state physics, simplifying the description of electron-nucleus interactions in crystalline solids. By replacing the full potential with an effective pseudopotential, it efficiently captures essential features, allowing for more manageable calculations. In this work, is to represent the band structures of 14 semiconductors Si, Ge, Sn, GaP, GaAs, AlSb, InP, GaSb, InAs, InSb, ZnS, ZnSe, ZnTe, CdTe, using pseudopotential method and compare the result with Cohen-Bergstresser, 1966.

2 Method

Computer program will be implemented using octave for band structure data calculation and python for visualization by following steps.

Initialization and Unit Conversion

Set as the reciprocal unit for conversion and kinetic energy scale.

Reciprocal Vectors Generation

Using equation (1.17), calculate unit reciprocal lattice vectors **g** and the length of it. The we generates reciprocal lattice vectors by iterating over a grid of nodes in reciprocal space, calculates their properties, filters them based on a cutoff radius, and updates relevant variables accordingly.

Construction and truncation of Hamiltonian in reciprocal space

Fourier coefficients are computed using equation (3.107) for each reciprocal lattice vector. Off-diagonal elements of the Hamiltonian are calculated based on conditions related to reciprocal lattice vectors **G**.

Diagonalization of Truncated Hamiltonian

This step contains calculating kinetic energy, diagonalizing the truncated Hamiltonian, and outputting the resulting band structure for further analysis and interpretation.

Data storage and visualization

Output file in **dat** type will be converted to **csv** file and will be handled with python.

3 Result and discussion

Below are the visualization of of band structures represent our calculation (left) and result of Cohen-Bergstresser (right). Comparison shows that there is a significant similarity between our simulation and the result from Cohen-Bergstresser of all cases. The minor disparities in the band shapes can be attributed to slight variations in the aspect ratio between our graphs and the reference graphs. Different colors represent different bands.

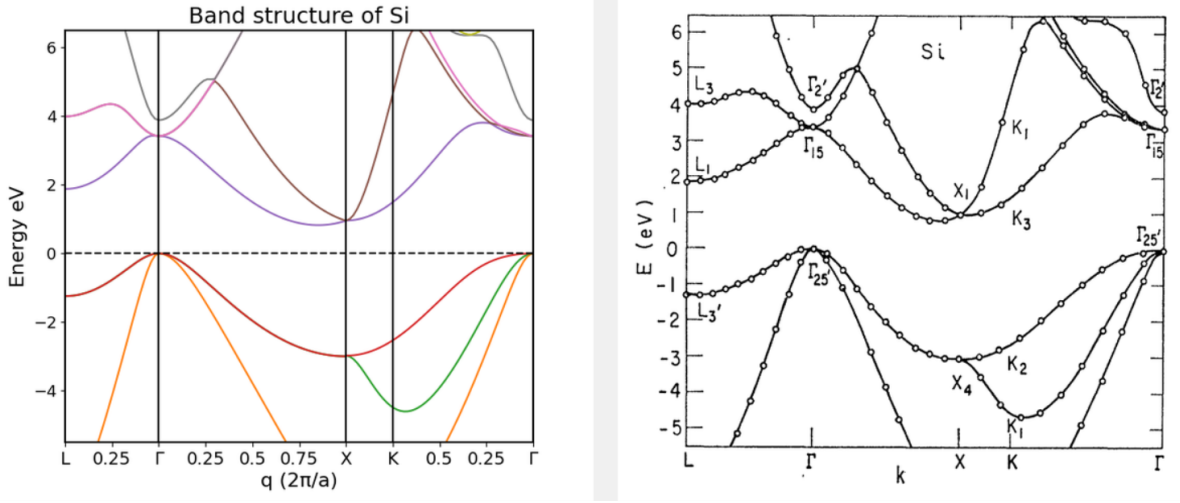

Figure 1: Band structure of Si

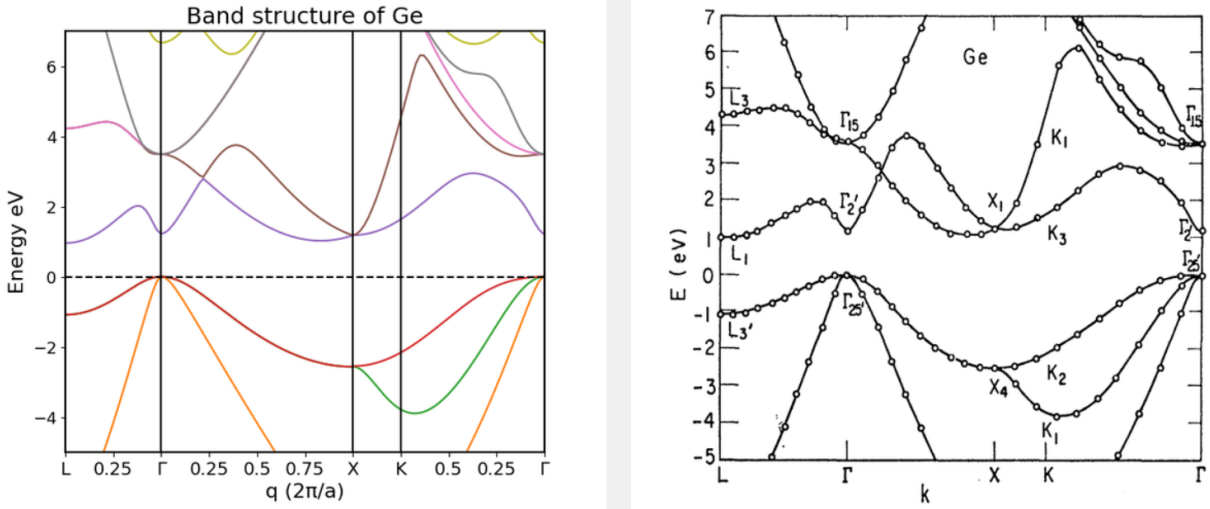

Figure 2: Band structure of Ge

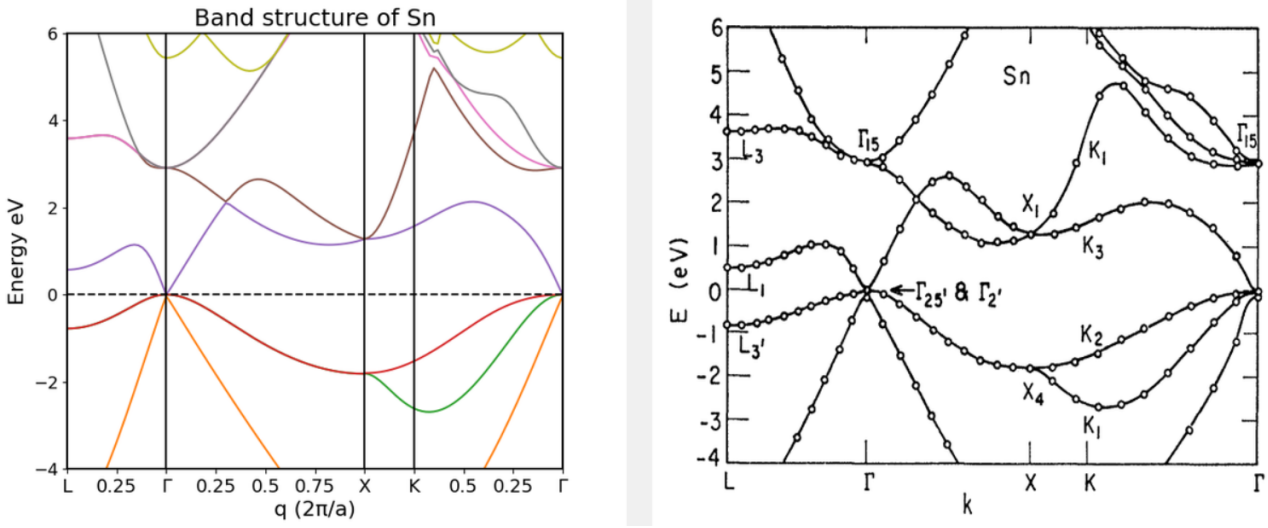

Figure 3: Band structure of Sn

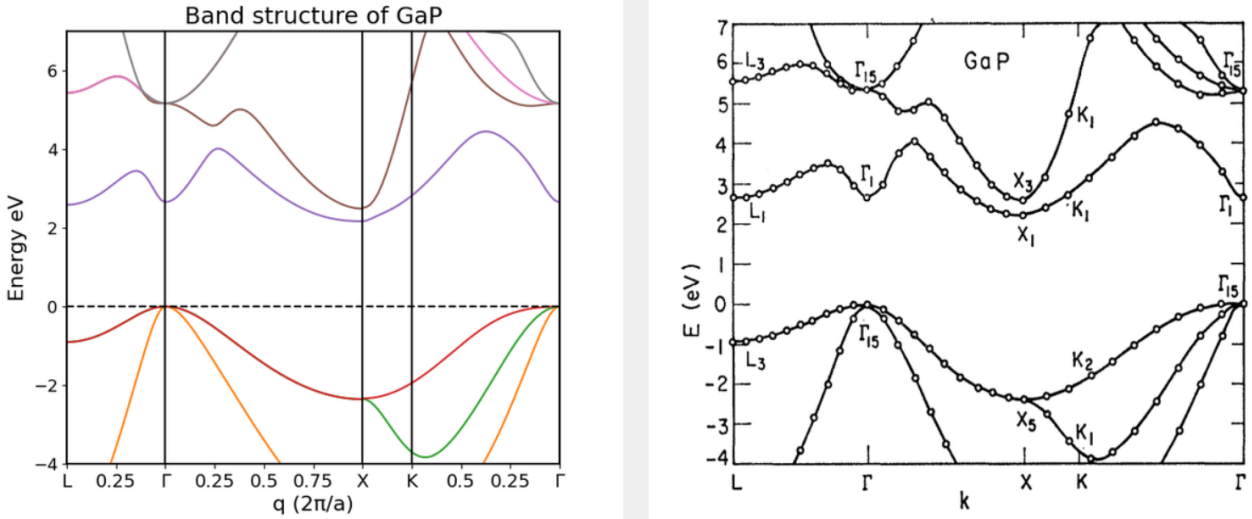

Figure 4: Band structure of GaP

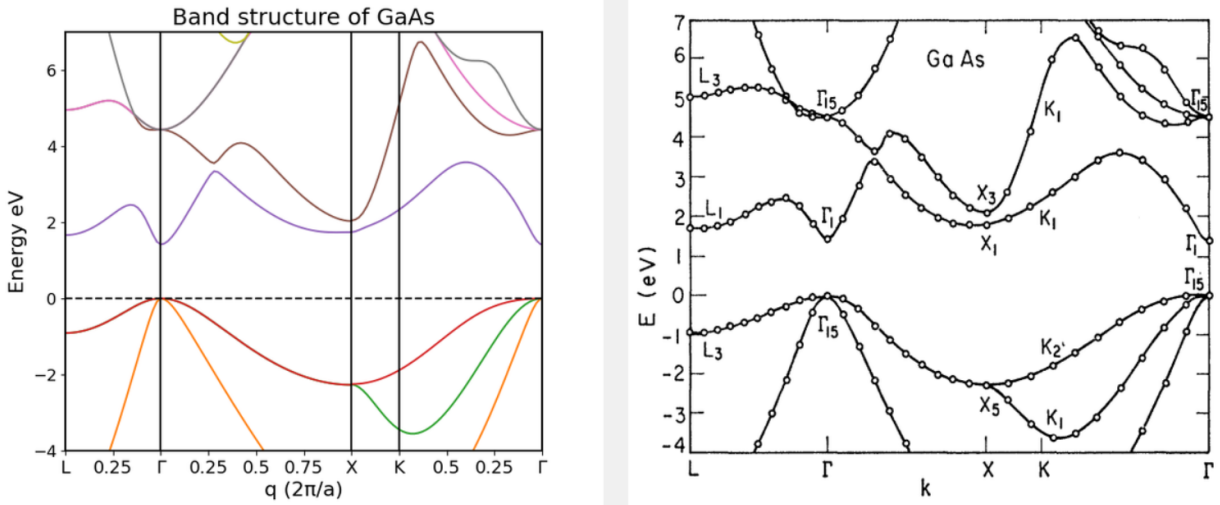

Figure 5: Band structure of GaAs

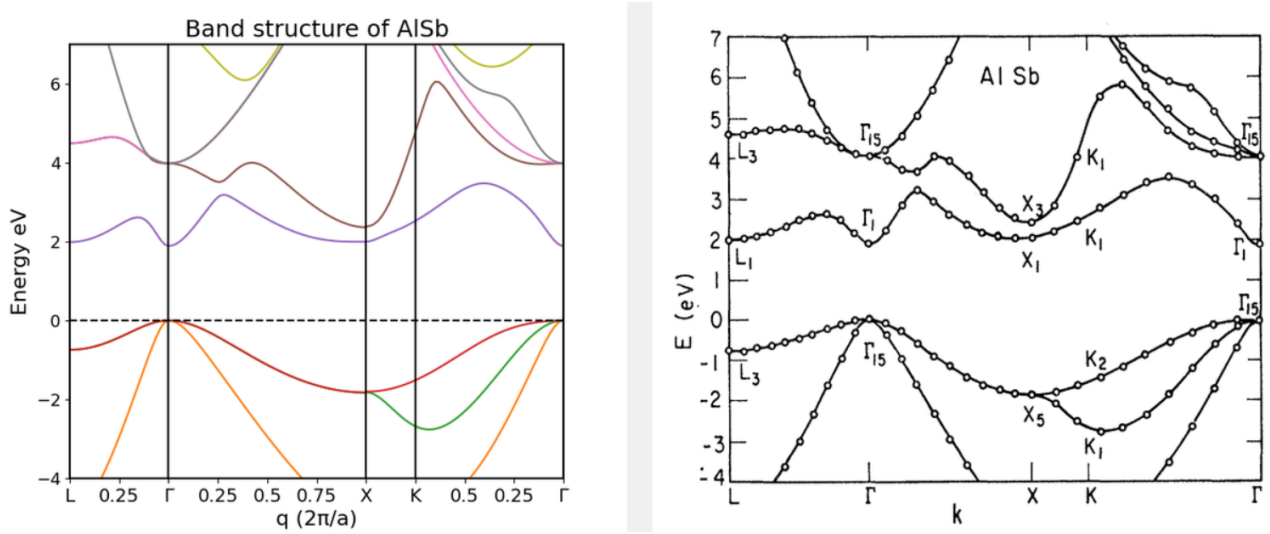

Figure 6: Band structure of AlSb

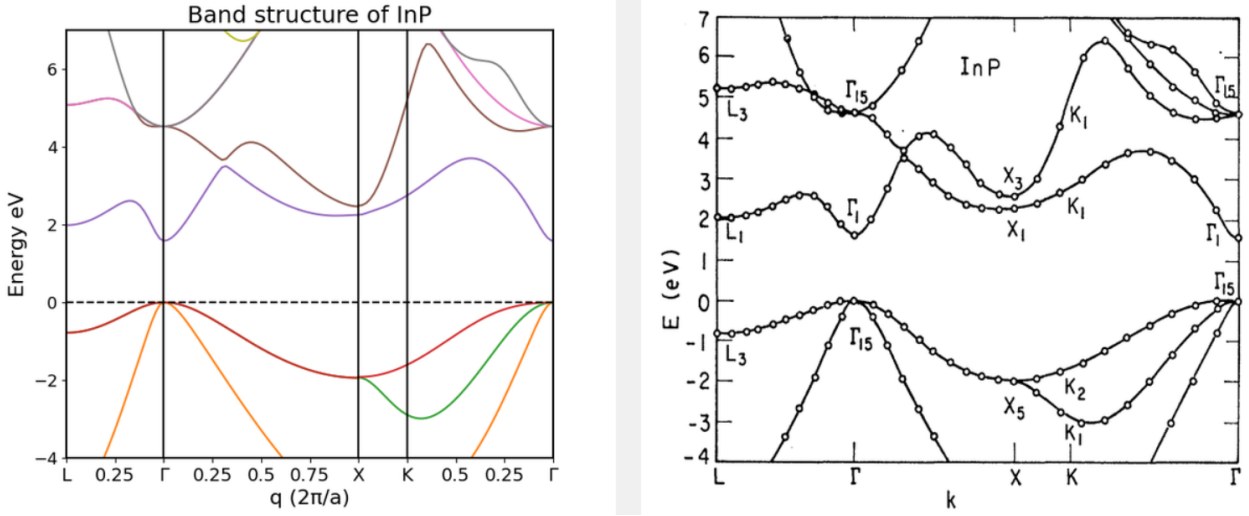

Figure 7: Band structure of InP

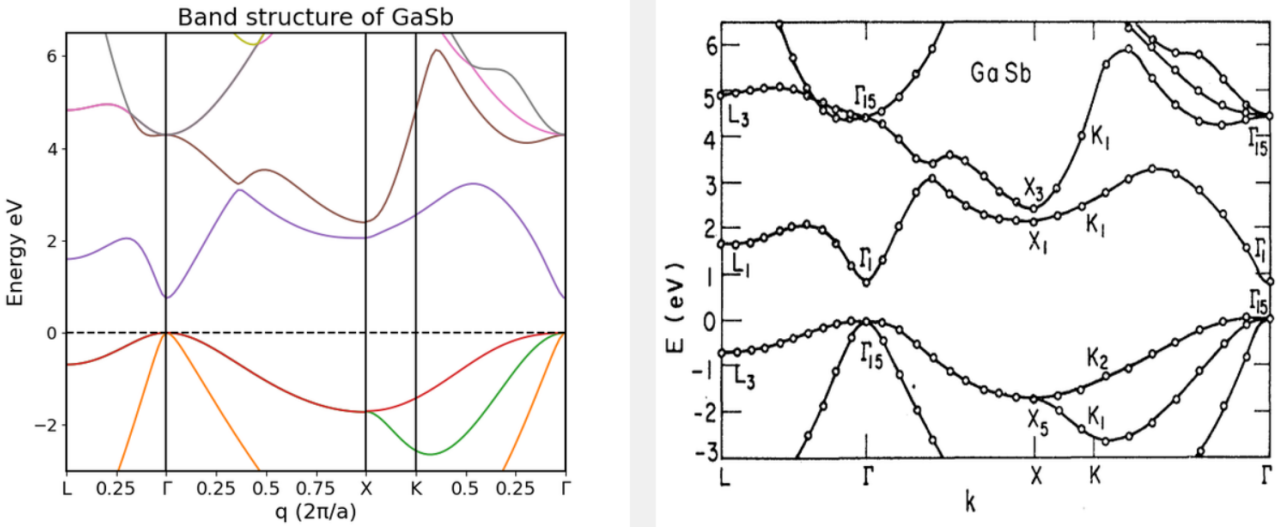

Figure 8: Band structure of GaSb

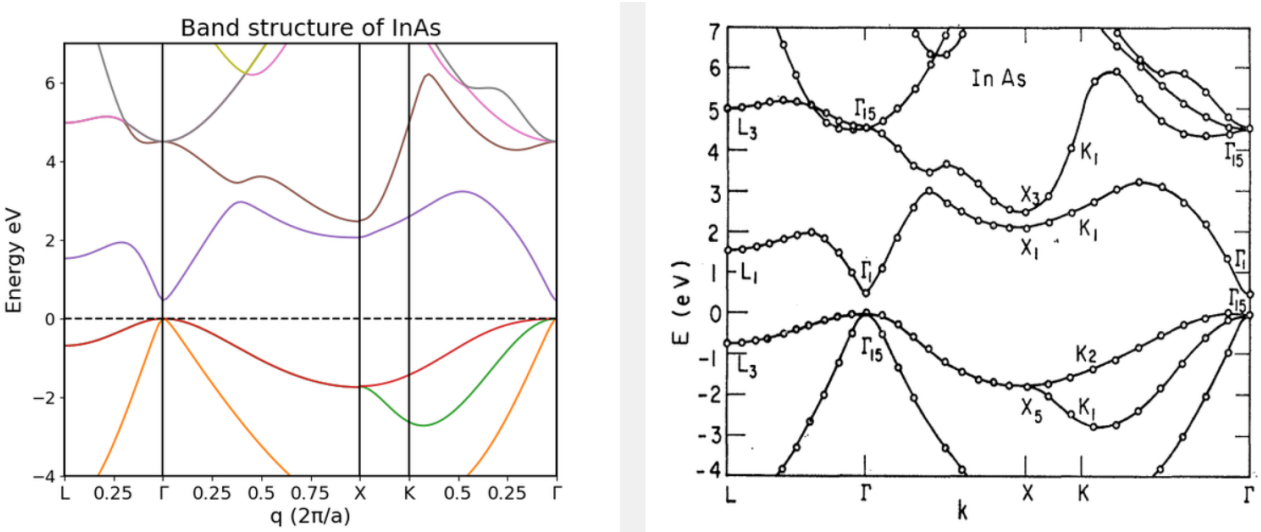

Figure 9: Band structure of InAs

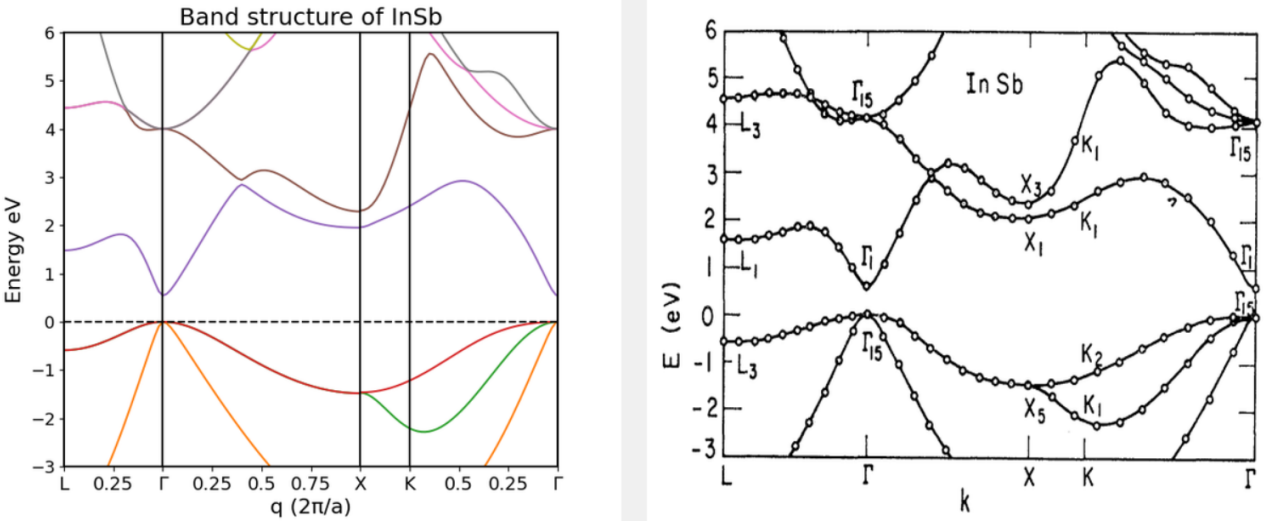

Figure 10: Band structure of InSb

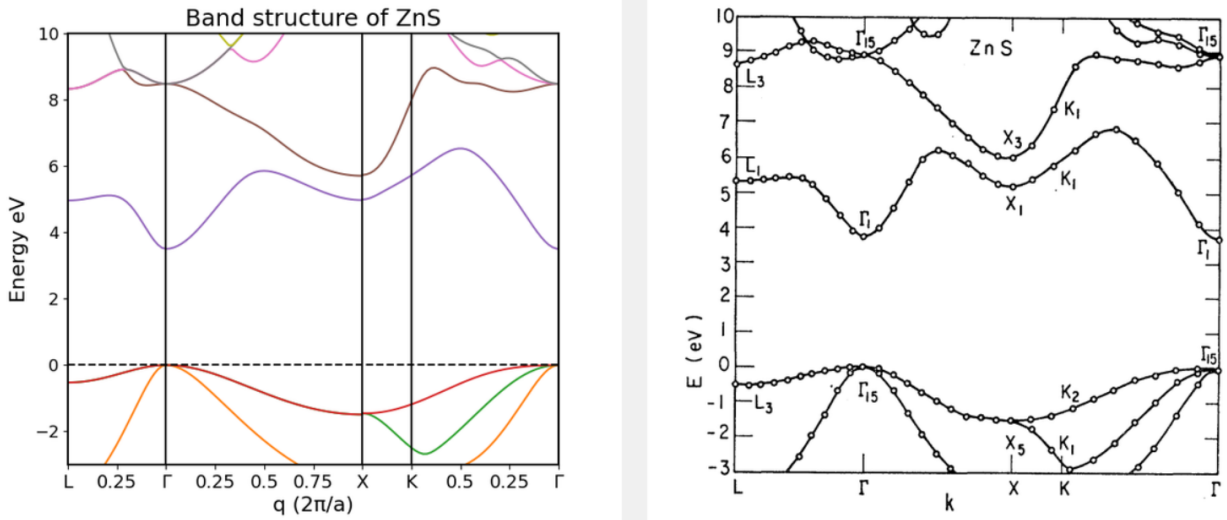

Figure 11: Band structure of ZnS

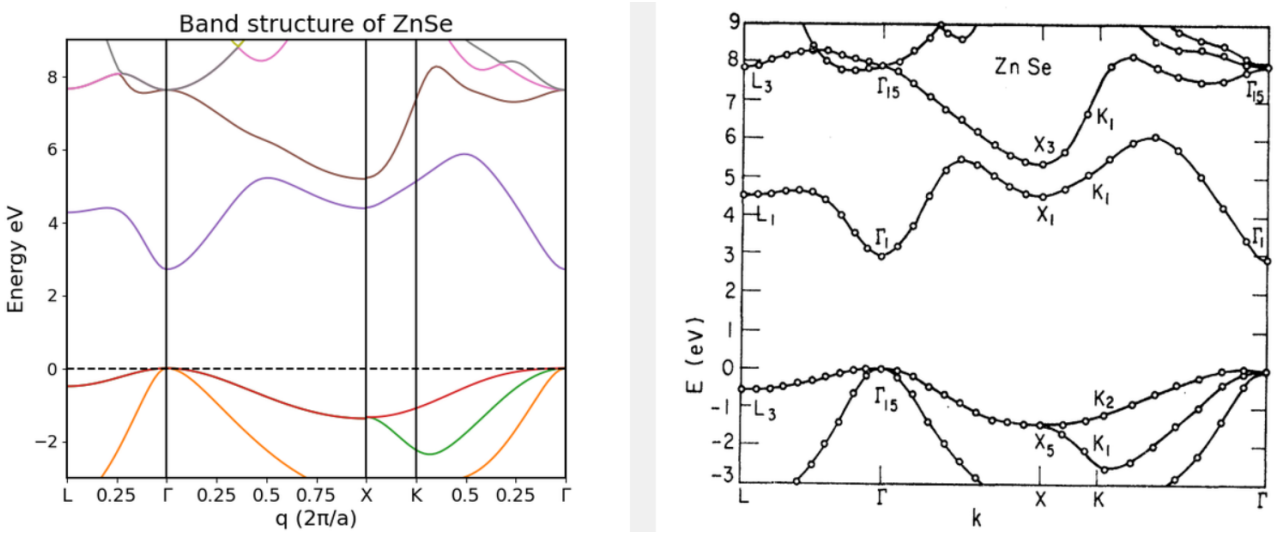

Figure 12: Band structure of ZnSe

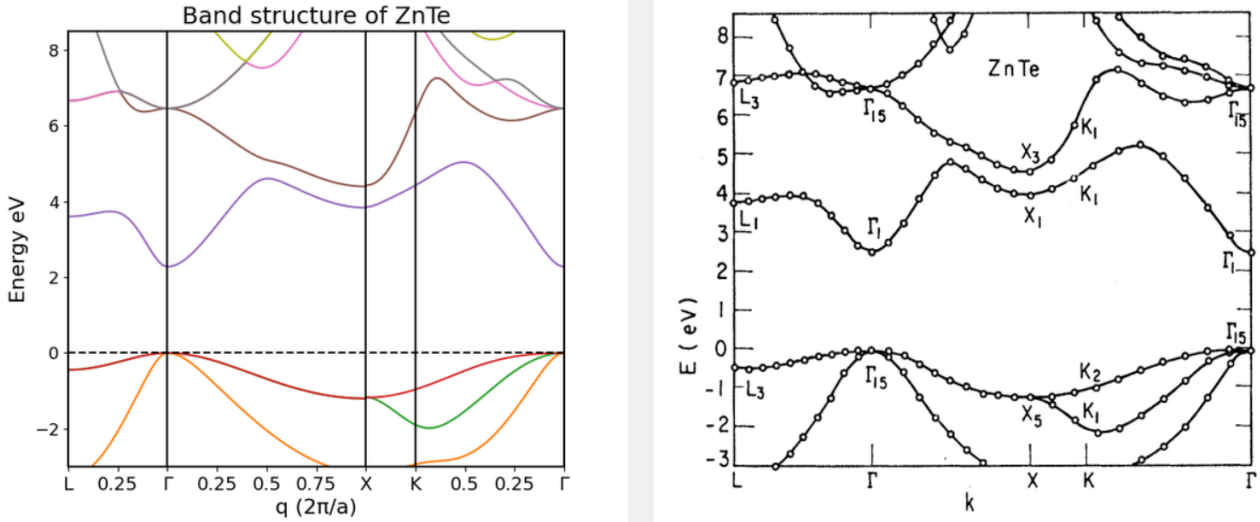

Figure 13: Band structure of ZnTe

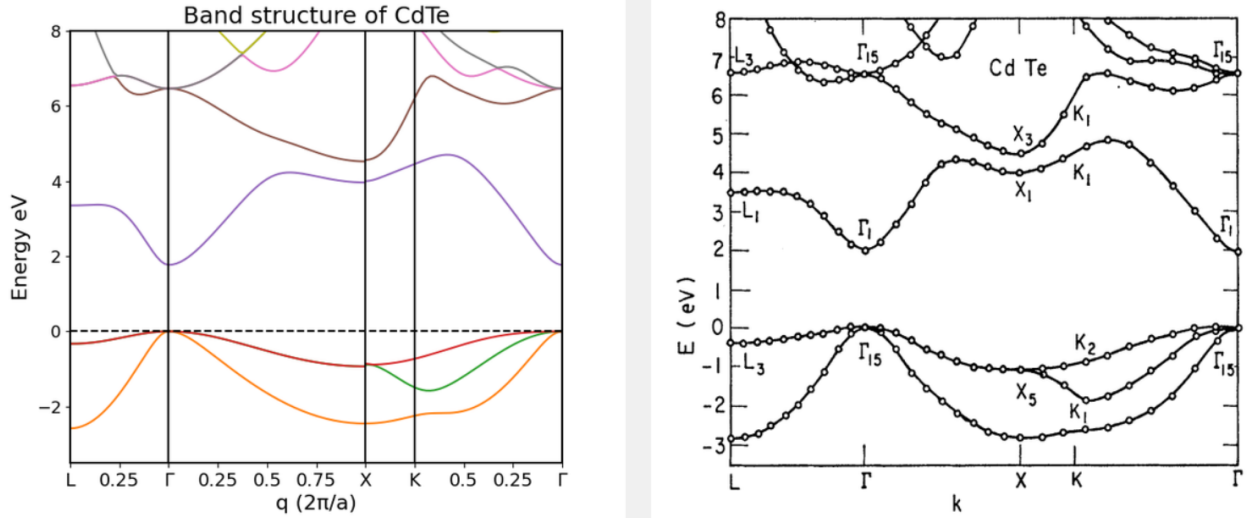

Figure 14: Band structure of CdTe