Computational Activity 4

Density of States and Band Structures

Objectives:

In this activity, you will

1) calculate the total density of states, atom-projected density of states, and orbital projected density of states of materials
2) calculate the electronic band structure of materials
3) write a written report of the results

Theory:

In analyzing the electronic properties of materials, one indispensable quantity to describe the electronic state of a material is the electronic density of states (DOS). It is simply the number of electron states with energies in the interval E and E + dE. There are several points that have to be considered in calculating the DOS. First, a large number of k points is necessary. Second, energies must be plotted not in terms of an absolute energy but instead relative to the Fermi energy, E_F, which is the energy of the highest occupied electronic state. Using the DOS, you can describe the material as being metallic, semiconductor, or insulator. Also, deeper analysis of the DOS can provide information on the hybridization of the orbitals and the nature of bonding between atoms.

A more nuanced view of a material's electronic structure is often possible by examining the material's band structure. The band structure represents the energy of the available electronic states along a series of lines in a reciprocal space that typically form a closed loop beginning and ending at the gamma point. Using band structure calculations, we can identify that bands that cross the Fermi level, calculate the direct and indirect band gap, among others.

Computational Model:

DFT calculations will be implemented using Quantum Espresso with exchange-correlation term described using the generalized gradient approximation (GGA) based on Perdew-Burke-Ernzerhof (PBE) functional. The interaction between ions and electrons will be described using the projector augmented wave (PAW) method. Plane wave basis sets will be employed with an energy cut-off of 600 eV. The surface Brillouin zone integrations will be performed on a grid of 8×8×8 Monkhorst-Pack k-points using Methfessel-Paxton smearing of σ=0.2 eV.

Method:

1) Set up the position of the atoms comprising the following materials:
    a. bcc Fe
    b. fcc Au
    c. Si Diamond Structure

    For this activity, use the lattice constants reported in the literature.
2) Calculate the electronic density of states and describe the electronic and magnetic state of the material.
3) Calculate the band structure of the materials and plot them side-by-side with the electronic density of states.
4) Compare the electronic properties of these materials by analyzing the DOS and band structure.

Results and Guide Questions:

Figure 1: Density of States and Band Structure of a BCC Fe.

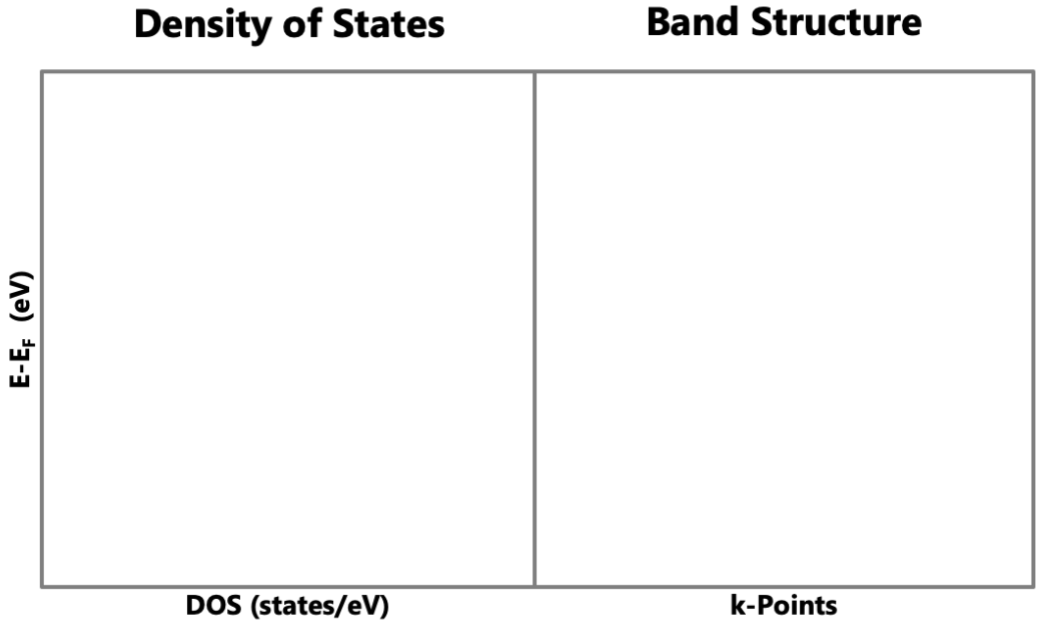


Figure 2: Density of States and Band Structure of an FCC Au.

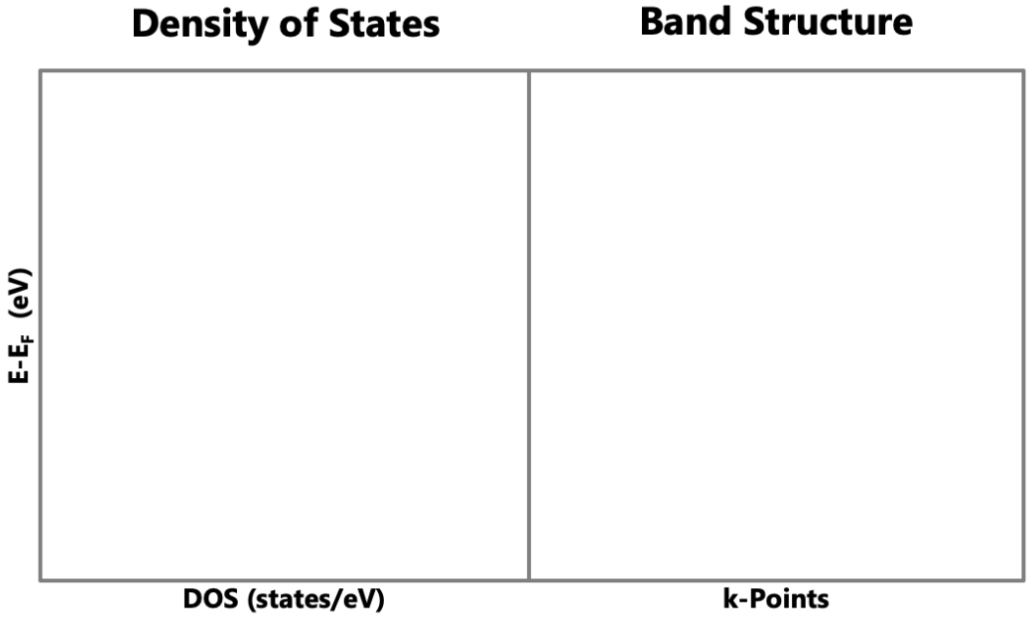
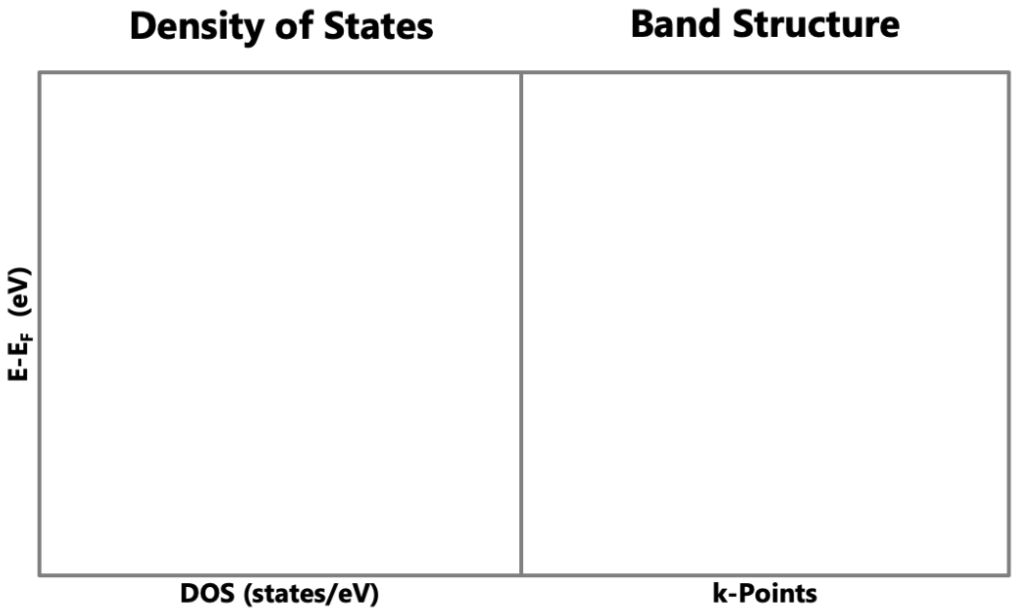


Figure 3: Density of States and Band Structure a Si Diamond



1) Describe the electronic and magnetic properties of a bcc Fe based on its density of states and band structure. Comment about spin-polarization and occupancy of the minority and majority spins.

2) Describe the electronic properties of an fcc Au. Comment about the amount of states that are occupied and unoccupied, and its possible relation to its reactivity.

3) Describe the electronic properties of a diamond Si. Comment about the presence of absence of electronic states in the Fermi level and its relation to the electronic properties of materials.

4) Among these materials, identify the ones that exhibit a metallic, insulating, and semiconducting properties. If the material is semiconducting, is the band gap direct or indirect?

5) Explain how you can determine the value of energy band gap from the DOS and band structure.

Conclusion: