MSE-423 **Exam** 02/02/2024

Submit only the final version of the answers inside the folded A3 sheet. Write your last name on the top left corner of each A4 sheet and sign the A3 sheet.

Question 1

Demonstrate that, for any 1-electron wavefunction $|\psi\rangle$, the expectation value of the energy $E[\{|\psi\rangle\}] = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}$ is always greater or equal to the ground state energy E_0.

Question 2

1. State what Bloch theorem is and under which assumptions it is valid.
2. Bloch theorem can be expressed in 2 forms. Choose one form and derive the other form from the previous one.
3. Prove Bloch theorem.

Exercise 1

Let us consider the CH_3Cl molecule (see Fig. 1).

1. Determine all the symmetry operations of CH_3Cl.
2. Verify that the group formed by the symmetry operations is closed with respect to multiplication.
   Hint: make the table of symmetry combinations. Do all combinations belong to the group?

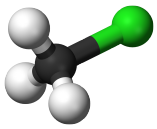

Figure 1: The CH_3Cl molecule.

Exercise 2

The electronic band structure and the density of states (DOS) are important properties that allow us to understand basic aspects of the behavior of materials. In the following, we will consider band structure plots and DOS from actual calculations.

1. The electronic band structure and the DOS of aluminium and copper are presented in Fig. 2. What is the Bravais lattice of Al? Of Cu? How many atoms are in the primitive unit cell for each material? Starting from the electronic configuration of the Al and Cu atoms, try to recognize which band structure refers to Al and which one refers to Cu and explain why. Match the DOS with the corresponding band structures. The figures are labeled "A", "B", "C", "D".
2. Consider the electronic band structure of three prototypical semiconductors, namely Si, Ge, GaAs (see Fig. 3). Which figure correspond to which material? Which of these semiconductors has a direct band gap and which one has an indirect band gap? The figures are labeled "1", "2", "3".
3. What is the wavelength of a photon whose energy equals the band gap of these materials? From the wavelength, determine the momentum of the photon. Estimate also the momentum of electrons with a wavevector at the X point. The lattice parameter for Ge, Si, and GaAs is $a \approx 5$ Å. Which of these materials will absorb the radiation with such a photon? Why? **In this question, you should only estimate order of magnitudes (e.g., $\frac{4.21*10^{-15}*3.14*10^{8}}{1.2} \approx 10*10^{-7}$).**
   (*Hint: In the absorption process, both energy and momentum should be conserved. You may find useful the following constants:* $h \approx 4.136*10^{-15}(eV*s)$, $c \approx 2.998*10^{8}(m/s)$)

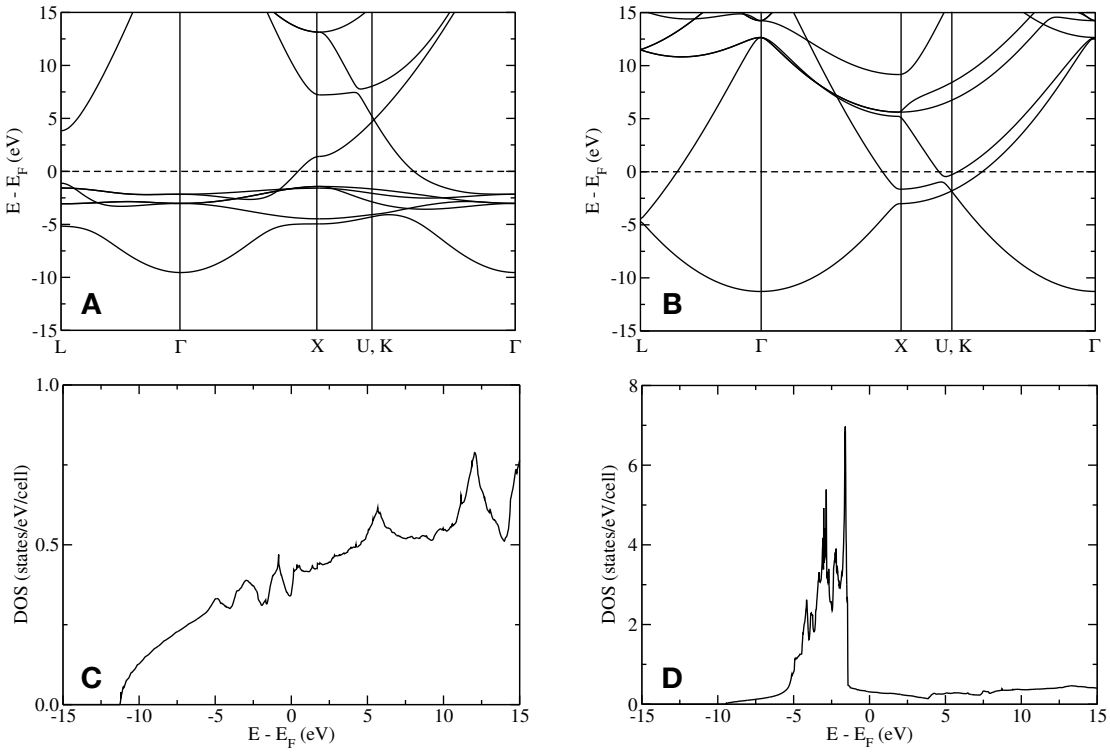

Figure 2: Electronic band structures (A,B) and density of states (DOS - C,D) for Al and Cu (in random order). E_F is the Fermi energy.

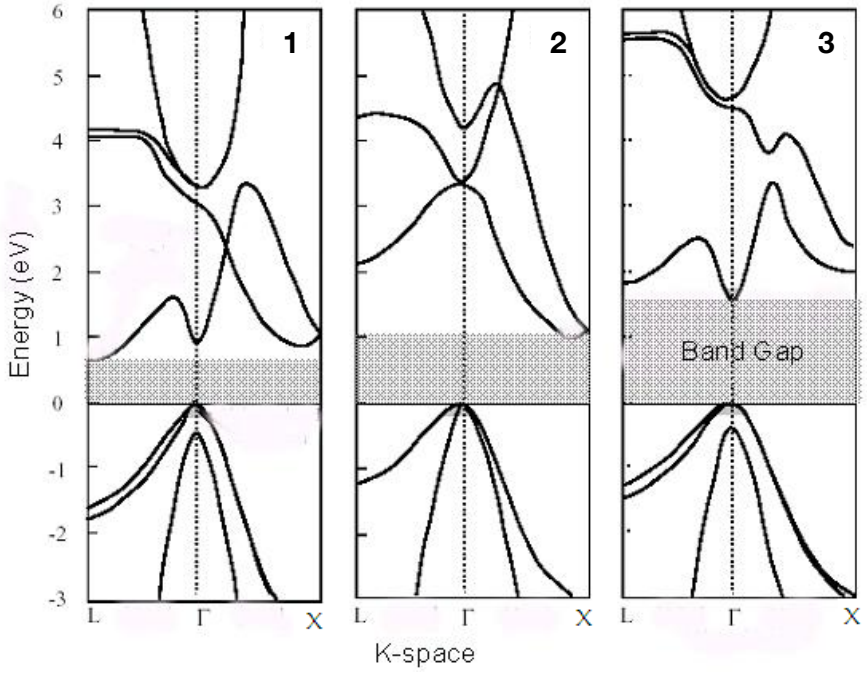

Figure 3: Electronic band structures of three semiconductors.

The End.