# Molecular and Solid State Physics

## Exam Jun 24, 2025

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| Name: | [redacted] |
| Mat. Nr: | |

### Additonal information

Be: 4 protons, O: 8 protons

$$\sum^{n} n = \frac{n(n+1)}{2}$$

## Question 1: Schrödinger equation (25 points)

Beryllium oxide (BeO) is a simple diatomic molecule which forms a covalent bond between both atoms.

a) The correct antisymmetric wavefunction can be written as a Slater determinant. How many entries (in total, i.e. including all core electrons) are in the Slater determinant for BeO? (30% of the points)

[redacted]

c) How many individual electron-electron repulsion terms are in this Hamiltonian? (It is ok to give an algebraic answer without calculating the final number). (15% of the points)

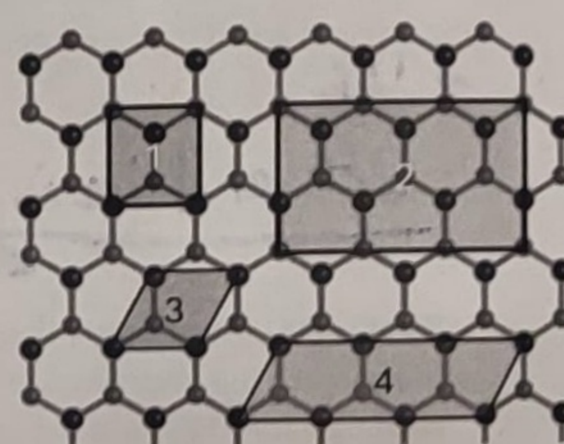
d) Using only the 2s orbitals for Be and the 2s and 2p orbitals for O, set up a term scheme for BeO. Assume that the 2s orbital of Be is at approximately the same energy as the 2p orbitals of O, and that the 2s orbitals of O are energetically much lower than the other orbitals. Is this molecule expected to be stable? (30% of the points)

e) **Bonus question**: How many molecular orbitals in this term scheme are $\pi$-orbitals? (15% of the points)

## Question 2: Crystal structure (25 points)

a) The pattern below shows the crystal structure of BN, a so-called 2D semiconductor, together with 4 potential unit cells (colored and labelled with numbers). Please mark whether the following statements are correct (c) or false. (10% for a correct answer, -10% for an incorrect answer: min 0%, max 60% of the total points).

[redacted]

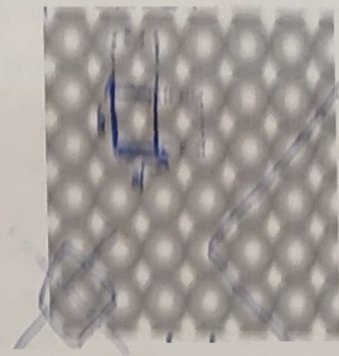



b) How many phonon bands are found for BN (using unit cell 3)? How many of these are acoustic phonons, how many are optical phonons? (30% of the points)

c) Explain, in your own words, how Miller indices for crystal planes are obtained. (10% of the points)

# Question 3: LEED (25 points)

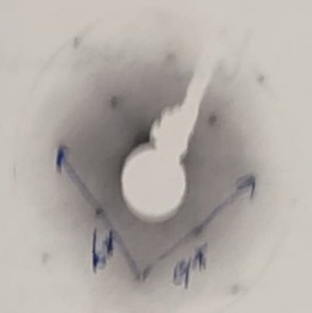
The sketch below is the surface which is obtained by a specific cut along a crystallographic direction of the Au crystal (FCC).



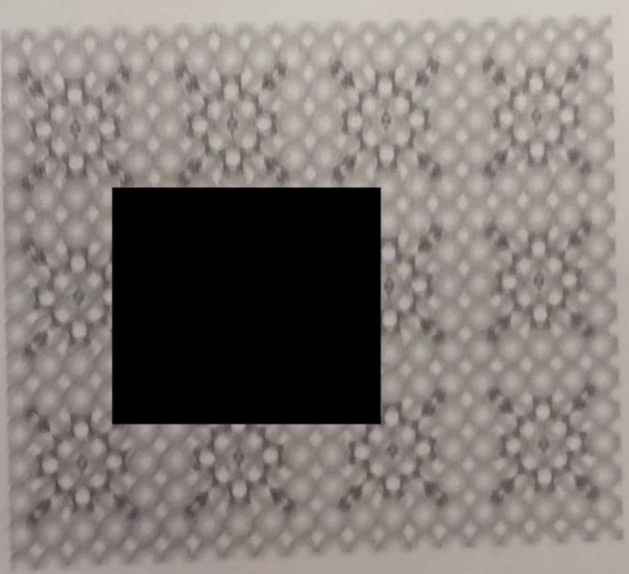
a) [redacted]

a) In the sketch above, draw (25% of the point):
   1. the [110] and [1$\bar{1}$0] crystallographic directions,
   2. a primitive unit cell and together with the primitive unit cell vectors.

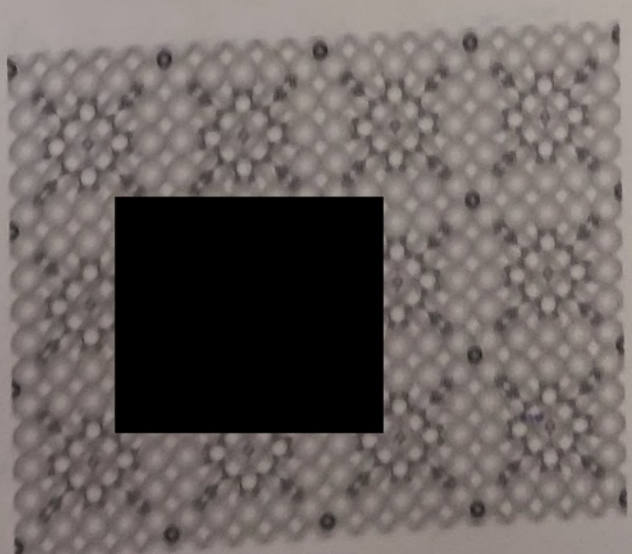
b) The Au surface shown at point 1) gives rise to the LEED pattern shown on the side, mark (on the figure) the first-order diffraction spot? (20% of the points)



c) We now deposit a molecule atop the Au surface. The molecules self-assemble in an ordered structure (see below) (15% of the points).
   1. Draw a new primitive unit cell.
   2. How many molecules there are in the primitive unit cell?

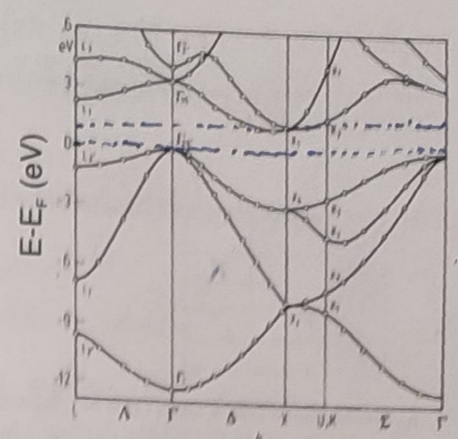


d) In a subsequent step of the experiment, we form a metal-organic framework, by deposition single Co atoms, which coordinate with the molecular side groups. The resulting structure is shown below (15% of the points).
   1. Draw the new unit cell
   2. How many molecules and Co atoms there are in the basis?



# Question 4: Seminconductors (25 points)

The picture below shows the band structure of a semi-conductor:




a. Indicate where the band gap is located. What type of band gap does the material have (direct or indirect)?
(20% of the points)

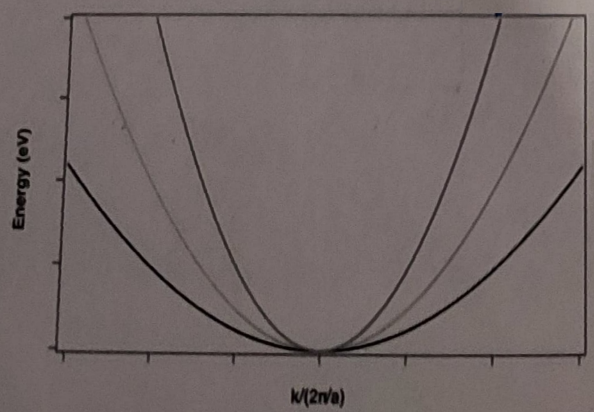
b. Can this semiconductor absorb light with photon energy $h\nu = E_g$ (where $E_g$ is the band gap energy)? Explain your reasoning. (20% of the points)

c. Would this semiconductor be suitable as an active material in an LED? Explain your reasoning. (10% of the points)

d. For semiconductors in general (not specific to the one shown here), why does the chemical potential typically lie near the middle of the band gap? Provide a qualitative explanation. (10% of the points)

e. Assuming now that the effective mass ratio at the top/bottom of the valence/conduction band is $\frac{m^*_h}{m^*_e} = 5$ ($m^*_h$ and $m^*_e$ are the hole and electron effective masses, respectively), in which direction would the chemical potential shift—towards the valence band maximum or the conduction band minimum? Explain your reasoning. (10% of the points)

f. Look at the graph below: (30% of the points)




1. Which band dispersion would lead to the highest effective mass? Which one the lowest? Explain your reasoning.

2. Assuming that this is the projection of the dispersion relation along a specific k-axis near the bottom of the conduction band in a 3D system, qualitatively sketch the density of states (DOS) for the **three dispersion relations**.