Question 4: Sommerfeld's model (25 points)

a. Which is the correct analytic expression of the density of states D(E) for a **2D electron gas**? (Hint, the density of states can be derived starting from its definition: $D(E) = \frac{dN}{dE}$)

[30% of the points]

a. $D(E) = \frac{\pi}{A}\sqrt{\frac{4m}{\hbar^2}}E^0$

b. $D(E) = \frac{2\pi}{A}\left(\frac{2m}{\hbar^2}\right)E^{1/2}$

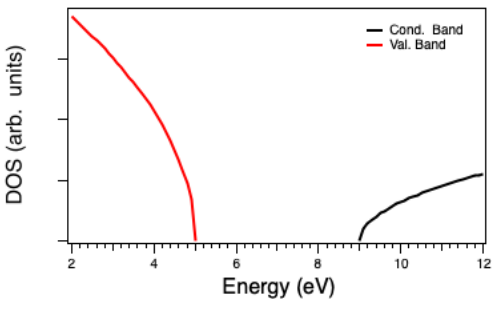
c. $D(E) = \frac{A}{2\pi}\sqrt{\frac{4m}{\hbar^2}}E^0$

d. $D(E) = \frac{A}{2\pi}\left(\frac{2m}{\hbar^2}\right)E^0$

e. $D(E) = \frac{\pi}{A}\left(\frac{4m}{\hbar^2}\right)E^0$

b. Below there is a plot of the density of states for a 3D Semiconductor close to the VB maximum / CB minimum. In this energy region, the electron bands can be approximated as renormalized parabolas, as described in the Sommerfeld's model.

[35% of the points]



- Mark the band gap in the graph
- At T>0, where would you draw the chemical potential? Should it be closer to the CB or the VB? Explain your reasoning.
- Draw the corresponding dispersion relation for the two DOS. Which one has the higher effective mass m*? Explain your reasoning.

c. For the Sommerfeld model, which of the following statements are true or false?
[max. 25%, min 0%, 5% for correct answers, -5% for wrong answers] **[25 % of the points]**

Statement	**t**	**f**
Electrons are described using Boltzmann statistics		
Every electron contributes equally to thermal excitation at low temperature.		
Within the Sommerfeld model, for every given **k** there is only one possible eigenvalue		
Decreasing the volume of the system while keeping the total number of electrons fixed increases the Fermi energy.		
For monovalent elements, the Fermi sphere is contained in the 1st BZ		

d. In your own words, explain the concept of work function and Fermi energy. **[10 % of the points]**

Molecular and Solid State Physics

Exam Jun 26, 2026

Name:
Mat. Nr:

Additonal useful information				
Element	**Z**		**x [°]**	**sin(x)**
H	1		0	0
C	6		30	0.5
N	7		45	0.707
O	8		60	0.866

Question 1: Schrödinger equation (25 points)

a) Below you find Hamiltonians for the hydroxyl radical (OH), the hydroxyl anion (OH^-), water (H_2O), and water cation (H_2O^+). Assign each Hamiltonian to the correct molecule. (Hint: An efficient way to approach this problem is to look at one type of term, such as the kinetic energy, in all equations, and decide which molecules it could fit) **[30%]**

$$\hat{H} = \sum_{\alpha\in A,B} \frac{-\hbar^2}{2M_\alpha}\nabla_\alpha^2 + \sum_{i=1}^{9} \frac{-\hbar^2}{2m_e}\nabla_i^2 + \sum_{\alpha\in A,B}\sum_{\beta>\alpha} \frac{1}{4\pi\epsilon_0}\frac{Z_\alpha e\cdot Z_\beta e}{|\vec{R_\alpha}-\vec{R_\beta}|} - \sum_{\alpha\in A,B}\sum_{i=1}^{9} \frac{1}{4\pi\epsilon_0}\frac{Z_\alpha e\cdot e}{|\vec{R_\alpha}-\vec{r_i}|} + \sum_{i=1}^{9}\sum_{j>i} \frac{1}{4\pi\epsilon_0}\frac{e\cdot e}{|\vec{r_i}-\vec{r_j}|}$$

$$\hat{H} = \sum_{\alpha\in A,B} \frac{-\hbar^2}{2M_\alpha}\nabla_\alpha^2 + \sum_{i=1}^{10} \frac{-\hbar^2}{2m_e}\nabla_i^2 + \sum_{\alpha\in A,B}\sum_{\beta>\alpha} \frac{1}{4\pi\epsilon_0}\frac{Z_\alpha e\cdot Z_\beta e}{|\vec{R_\alpha}-\vec{R_\beta}|} - \sum_{\alpha\in A,B}\sum_{i=1}^{10} \frac{1}{4\pi\epsilon_0}\frac{Z_\alpha e\cdot e}{|\vec{R_\alpha}-\vec{r_i}|} + \sum_{i=1}^{10}\sum_{j>i} \frac{1}{4\pi\epsilon_0}\frac{e\cdot e}{|\vec{r_i}-\vec{r_j}|}$$

$$\hat{H} = \sum_{\alpha\in A,B,C} \frac{-\hbar^2}{2M_\alpha}\nabla_\alpha^2 + \sum_{i=1}^{10} \frac{-\hbar^2}{2m_e}\nabla_i^2 + \sum_{\alpha\in A,B,C}\sum_{\beta>\alpha} \frac{1}{4\pi\epsilon_0}\frac{Z_\alpha e\cdot Z_\beta e}{|\vec{R_\alpha}-\vec{R_\beta}|} - \sum_{\alpha\in A,B,C}\sum_{i=1}^{10} \frac{1}{4\pi\epsilon_0}\frac{Z_\alpha e\cdot e}{|\vec{R_\alpha}-\vec{r_i}|} + \sum_{i=1}^{10}\sum_{j>i} \frac{1}{4\pi\epsilon_0}\frac{e\cdot e}{|\vec{r_i}-\vec{r_j}|}$$

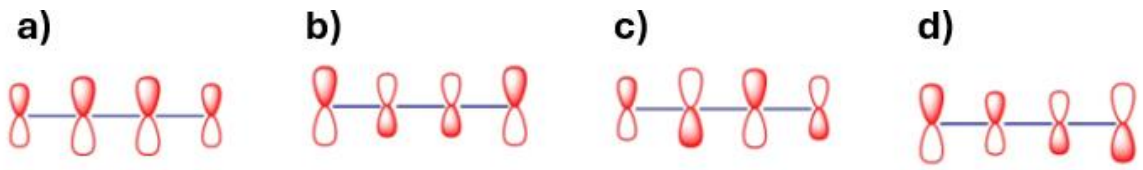
$$\hat{H} = \sum_{\alpha\in A,B,C} \frac{-\hbar^2}{2M_\alpha}\nabla_\alpha^2 + \sum_{i=1}^{9} \frac{-\hbar^2}{2m_e}\nabla_i^2 + \sum_{\alpha\in A,B,C}\sum_{\beta>\alpha} \frac{1}{4\pi\epsilon_0}\frac{Z_\alpha e\cdot Z_\beta e}{|\vec{R_\alpha}-\vec{R_\beta}|} - \sum_{\alpha\in A,B,C}\sum_{i=1}^{9} \frac{1}{4\pi\epsilon_0}\frac{Z_\alpha e\cdot e}{|\vec{R_\alpha}-\vec{r_i}|} + \sum_{i=1}^{9}\sum_{j>i} \frac{1}{4\pi\epsilon_0}\frac{e\cdot e}{|\vec{r_i}-\vec{r_j}|}$$

b) Water (H_2O), Ammonia (NH_3) and methane (CH_4) are all *isoelectronic*, i.e. have the same number of electrons (10 electrons in total, of which 2 are core electrons and irrelevant for this question). Explain how you can use the valence shell electron pair repulsion model (VSEPR) to determine the approximate geometry of these three molecules. What would their geometry look like (sphere, cube, pyramid, etc.) ? **[15% for the concept, 5% for the geometry]**

c) Which of the following statements are true or false? **[max. 20%, 5% for correct, -5% for wrong answers, min 0%]**

Statement	**t**	**f**
The Schrödinger equation has an infinite number of solutions		
When neglecting electron-electron interaction, the total energy is given by the sum over all energies of occupied orbitals		
The many-electron wave function is often given as a Slater determinant, because it enforces the anti-symmetry of the wave function		
A Slater determinant is an exact solution to the many-electron Schrödinger equation		

d) How is the orbital energy of a molecular orbital related to the number of nodes in the wave function? Below you find a side view of the 4 π-orbitals of 1,3-butadiene (CH_2=CH-CH=CH_2). Order these orbitals according to their energy. Look at orbital (d): With respect to which bonds is this orbital bonding, with respect to which bonds is this orbital antibonding? **[30%]**



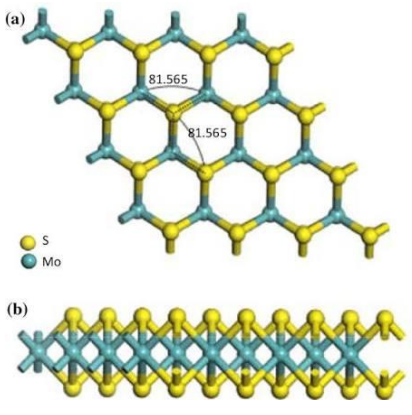
Question 2: Crystal structure (25 points)

a) Polonium crystallizes in a simple cubic crystal structure with a single atom in the unit cell at $\boldsymbol{R_{Po}}$ = (0,0,0) and a lattice constant of a ≈ 3.14 Å. *Sketch* the reciprocal lattice for polonium and indicate the length of the reciprocal lattice vectors (hint: An actual calculator is not required for this question). **[35%]**

b) How does the Bravais lattice type and the reciprocal lattice change if the basis is instead a single atom at $\boldsymbol{R_{Po}}$ = (a/2, a/2, a/2)? **[15%]**

c) Assume we are performing a diffraction experiment with neutrons (|k| = 2 $Å^{-1}$) that hit Polonium (100) at an angle of 30°. Will we observe scattering? Explain why or why not. (Hint: The question can be solved both in real and in reciprocal space). **[25%]**

d) The image below is a top and side view of a single layer MoS_2. It is a so-called 2D-material, meaning that it is a crystal (has translation periodicity) in two dimensions, but consists only of a single layer (of finite thickness). Which of the following statements are true or false **[max. 25%, 5% for correct, -5% for wrong answers, min 0%] [25%]**



Statement	t	f
The primitive 2D unit cell is hexagonal		
The primitive unit cell contains 2 inequivalent Mo and 4 inequivalent S atoms		
The phonon band structure (of the primitive cell) contains only acoustic phonons		
It is possible to construct a valid *face-centered rectangular* unit cell, which would be larger than primitive unit cell (not counted after exam)		
When choosing a larger unit cell, the mass density also becomes larger		

Question 3: The Bloch theorem (25 points)

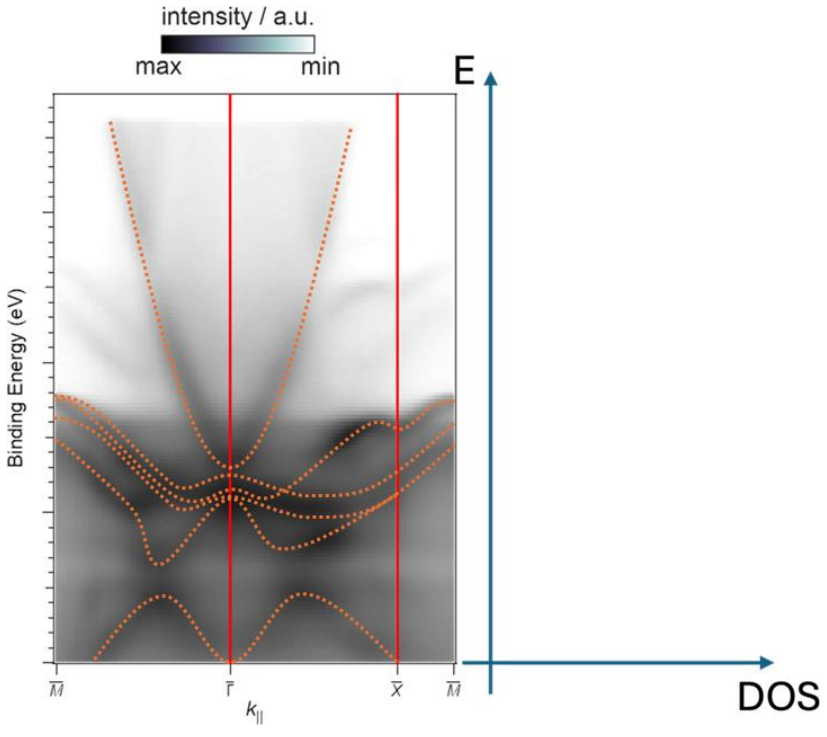
a) State the Bloch theorem. You can choose the main or the alternative formulation. Please be careful with the wording. **[30%]**

b) Prove that the following function: $\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \phi(\boldsymbol{r} - \boldsymbol{R})$, which is an ansatz used in the tight binding model, is a Bloch wavefunction (i.e. it satisfies the Bloch's theorem). [**25 %]**

c) Which of the following statements are true or false [max. 25%, min 0%, 5% for correct, -5% for wrong answers]**[25%]**

Statement	t	f
The Bloch wavefunction must have periodicity of the lattice		
In the reduced zone scheme, the crystal band structure is mapped in the 1st BZ		
As a result of the Bloch theorem, for every given **k** there is only one possible eigenvalue		
In the Bloch's Hamiltonian the position of the nuclei is frozen.		
The crystal momentum is an eigenstate of the momentum operator		

d) The image below is a band structure measurement from a material measured with photoemission. **Photoemission only probes occupied states**. You should only focus on the sharp bands and ignore the diffused background: the dashed orange lines serve as guide to the eye. $\overline{M}$, $\overline{\Gamma}$ and $\overline{X}$ are high symmetry points of the Brillouin Zone. **[20 %]**



- In the empty graph on the side, qualitatively draw the corresponding DOS.
- Mark the position Fermi Level.
- Is this a metal or an insulator? Explain your reasoning

- Looking at the band dispersion, estimate how many valance s, p and d-electrons per unit cell are in the system. Justify your answer.