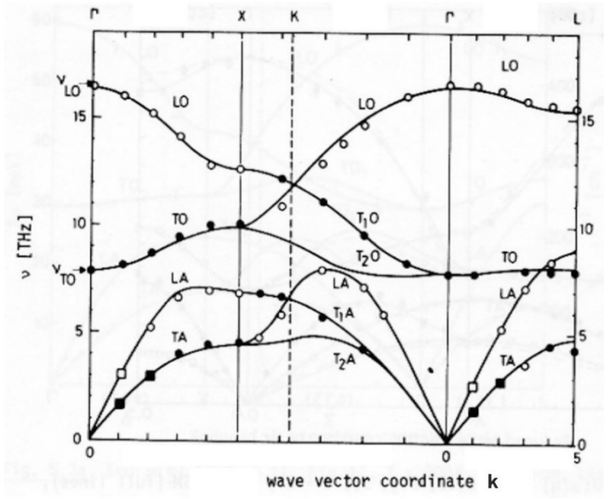
problem 3

Consider a crystal with a size of 1cm x 1cm x 1cm. The crystal structure is face centred cubic with two atoms within the primitive unit cell and with a lattice constant of a = 5 Å. A sketch of the phonon dispersion relation is given below.

a) How many acoustic branches exists?
b) How many phonon modes with different energies can be assigned to a single wavevector k.
c) Calculate the sound velocity for the transversal modes; use the figure below and take $\overline{\Gamma X} = \frac{2\pi}{a}$.
d) Use the density of states $D(k) = \frac{3k^2}{2\pi^2}$ and calculate D(λ). D(λ) is the density of states as a function of the wavelength λ.
e) How many phonon states are within the wavelength range of 1 µm to 10 µm



Re-examination / Molecule and Solid State Physics / 14 September 2020

Name / student ID number:

tutorial group (Egger / Hadley / Kamencek / Resel / Schwendt):

Five credits are possible for each sub-problem (a … e), total maximum: 100 credits

Results	a	B	c	d	E	Subtotal
problem 1						
problem 2						
problem 3						
problem 4						
					total	

problem 1

Consider a molecule HF formed by a fluorene atom and a hydrogen atom. The fluorene atom consists of nine protons (and ten neutrons) in the atomic nucleus (mass m_F at position r_F) paired with nine electrons (mass m_e at positions r_1, … r_9) in the 1s, 2s and 2p state. The hydrogen atom has one proton in its atomic nucleus (mass m_p at position r_p) paired with one electron (mass m_e at position r_{10}) in the 1s shell.

a) The first question is related to the many particle Hamiltonian for the molecule HF. Write down all parts where the single electron of hydrogen is involved. Please use the proper masses (m_F, m_p, m_e), their charges (±e, +9e) and their positions (r_F, r_p, r_1, … r_9) of the involved particles.

b) Write down the molecular orbital Hamiltonian for a single electron for the molecule HF. How many terms does this Hamiltonian consists of? Ignore Slater rules and use Z = 9.

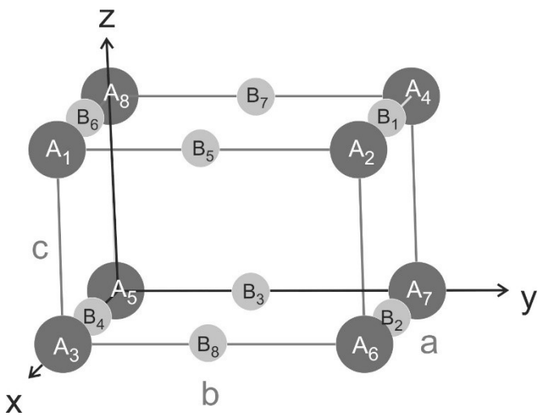
c) A molecular orbital wavefunction (MO-wavefunction) can be constructed for the Hamiltonian given in c) by a linear combination of atomic orbitals. Write down an Ansatz for the MO-wavefunction using atomic orbitals.

d) How many molecular orbitals would be obtained by using the Ansatz MO-wavefunction you gave in part (c)?

e) How many molecular orbitals would be occupied by using your Ansatz MO-wavefunction?

problem2

Consider a tetragonal crystal structure with a = b = 4 Å, c = 3 Å and α = ß = γ = 90°. A sketch of the crystallographic unit cell is given below with dark grey spheres as atoms of type A and light grey spheres as atoms of type B. The atoms A are located at the edges of the unit cell, the atoms B are located at the side edges of the a and b axes.



a) How many atoms A and how many atoms B are within the crystallographic unit cell?

b) The tetragonal unit cell is a primitive Bravais lattice (one lattice point per unit cell). Which atoms are the basis of the unit cell? Please denote the atoms with their respective labels (A_1, A_2, B_1, B_2, etc..)

c) Draw the arrangement of the atoms within the crystallographic plane with the Miller indices h = 0, k = 1, l = 1. Give two characteristic distances between atoms A within your drawing.

d) Calculate the reciprocal lattice vector $\vec{G}_{110}$ as well as the length of G_{110}.

e) Calculate the structure factor of the 110 Bragg peak. Use $f_A(G_{110})$ and $f_B(G_{110})$ as the atomic scattering factors of atoms A and B, respectively.

problem 4:

Consider the free electrons within a three-dimensional crystal structure with an electron density of n = $9*10^{28}$ m^{-3}. The density of states D(E) is sketched below by $D(E)[m^{-3}J^{-1}] = 10^{66}[m^{-3}J^{-2}] * E[J]$.

a) Is this a metal / semiconductor / insulator? Why?
b) Determine the Fermi energy (chemical potential µ at a temperature T = 0 Kelvin).
c) Give the density of the occupied electronic states D(E) f(T) as a function of energy at a temperature of 300K.
d) How would the internal energy be calculated at T = 300 K?
e) How would the chemical potential be calculated at T = 300 K?