Utrecht University
Exam Structure of Matter
Tuesday, March 6th, 2018
Time: 13:30 - 16:30

Name and student number: _____

Good luck!

- Please pay attention to your hand-writing. If we cannot read your answers, we cannot award points.
- In your answers, do not immediately start with equations. Also draw conclusions from the calculations you have done.
- Calculators, graphical or otherwise, are not allowed.
- Please note that you can earn a maximum of 61 points.
- Not each question is worth the same number of points.
- Questions have been ordered by subject, not by difficulty. Suggestion: save the most difficult/time consuming questions for last.
- The following relations might be helpful:

$$\cos(2a) = 2\cos^2 a - 1$$
$$\cos(a+b) = \cos(a)\cos(b) - \sin(a)\sin(b)$$
$$\cos(a-b) = \cos(a)\cos(b) + \sin(a)\sin(b)$$
$$e^{ik} + e^{-ik} = 2\cos(k)$$
$$\int_{-\infty}^{\infty} f(x)\delta(x-x_0)\,dx = f(x_0)$$

Question 1: **Atomic Physics** ..... *10 points*

(a) (2 points) Give the electron configuration of Si ($Z = 14$)

(b) (2 points) Give the electron configuration of Ag ($Z = 47$)

(c) (6 points) Electronegativity is a property of atoms that describes the tendency of an atom to attract electron density towards itself. An atom's electronegativity is affected by both its atomic number and the distance at which its valence electrons reside from the nucleus. The higher the associated electronegativity number, the more an element or compound attracts electrons towards it. Describe how the electronegativity changes when crossing a period of the periodic table, as well as how it changes when going down a group **AND** explain.

Question 2: **Molecular Physics 1** ..... *12 points*

Vision begins with the photoisomerization of retinal (one of the many forms of vitamin A). The reaction is shown in Figure 1 below. Upon adsorption of a photon, there is a rotation about one of the C-C double bonds. For the aficionados: When the 11-cis-retinal chromophore absorbs a photon it isomerizes from the 11-cis state to the all-trans state. In this question, you will explore how adsorption of a photon can lead to such an isomerization.

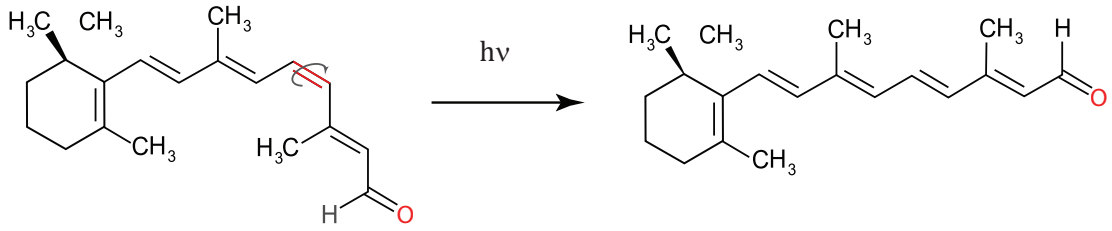

Figure 1: The first step in vision is a chemical reaction, the photoisomerization of retinal.

Consider the simplest model system with C-C double bonds: ethylene (C_2H_4). Rotation over the C-C double bond involves breaking the π-bond, which is energetically unfavorable. Consequently, C-C double bonds, i.e. C atoms bound by a σ and a π orbital are structurally rigid and for all intents and purposes rotations about such bonds do not occur at room temperature.

For ethylene (and retinal) to isomerize, the π-bond therefore has to be broken, such that part of the molecule can (freely) rotate about the remaining σ bond. Within the framework of Hückel calculations this implies a bond order of zero. The bond order between atoms i and j, is given by:

$$b = \sum_{k=1}^{K} n_k c_i^k c_j^k \tag{1}$$

n_k indicates the number of electrons in orbital k. The sum runs over all occupied orbitals. Assume that in your Hückel calculation you only have to take into account the double bond that undergoes isomerization.

(a) (5 points) Give the matrix corresponding to the simplified retinal system, compute the energies of the molecular orbitals **AND** draw the MO diagram.

(b) (2 points) What happens physically upon adsorption of a photon?

(c) (5 points) Calculate the π bond order in the ground and excited state of ethylene. Comment on the feasibility of isomerization.

Question 3: **Molecular Physics 2** ..... *5 points*

(a) (2 points) Describe the concept of orbital hybridization.

(b) (3 points) Consider the molecules shown in Figure 2. C, H and N atoms are indicated in black, white and blue, respectively. N has atomic number $Z = 7$. For each molecule, indicate if the N atom is hybridized, and if so, how. **Hint**: consider the number of valence electrons. All of these need to be accommodated.

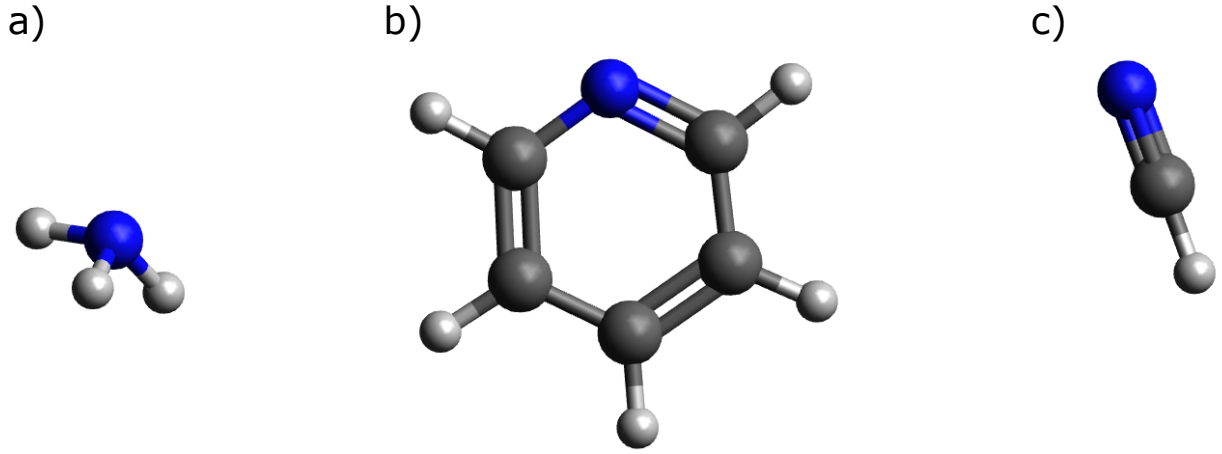

Figure 2: Three-dimensional form of 3 nitrogen containing molecules.

Question 4: **Condensed Matter Physics** ..... *26 points*

You will perform a tight-binding calculation of crystalline Lithium. Only interactions with nearest neighbors have to be taken into account. Each atom contributes one $2s$ orbital and one electron.

Lithium forms crystals with a body centered cubic (bcc) Bravais lattice, see Figure 3. The primitive lattice vectors for a bcc lattice with lattice constant a are

$$\boldsymbol{a_1} = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z}) \tag{2}$$

$$\boldsymbol{a_2} = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z}) \tag{3}$$

$$\boldsymbol{a_3} = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z}) \tag{4}$$

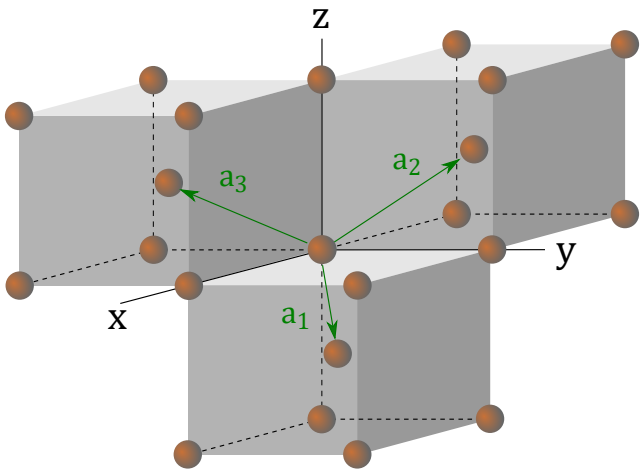

Figure 3: Part of a lithium crystal. Unit vectors defined above are indicated.

(a) (5 points) Determine the reciprocal space unit cell of Lithium

(b) (2 points) The Wigner-Seitz cell in reciprocal space has a special name. What is that name?

(c) (3 points) How many nearest neighbor atoms does each Lithium atom have? Indicate them in a drawing.

(d) (12 points) Show that a nearest-neighbor tight-binding calculation results in the following dispersion relation

$$E(\boldsymbol{k}) = \alpha - 8\beta \cos\left(\frac{k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) \cos\left(\frac{k_z a}{2}\right) \tag{5}$$

(e) (4 points) Given the dispersion relation, explain if lithium is a metal, semiconductor or insulator. Include the term *Fermi level* in your answer.

Question 5: **Soft Matter** ..... *8 points*

(a) (3 points) Describe the differences between a crystal, a quasicrystal and an amorphous material.

(b) (2 points) The Lennard Jones potential which is used to approximate interatomic interactions is given in Equation 6.

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \tag{6}$$

Give the names or briefly describe the phenomena which give rise to the two terms in Equation 6.

(c) (3 points) Figure 4 shows radial distribution functions for a system of Lennard Jones particles in different configurations. Describe the structures of the three different configurations and justify your answer with reference to the features of the g(r) in each case.

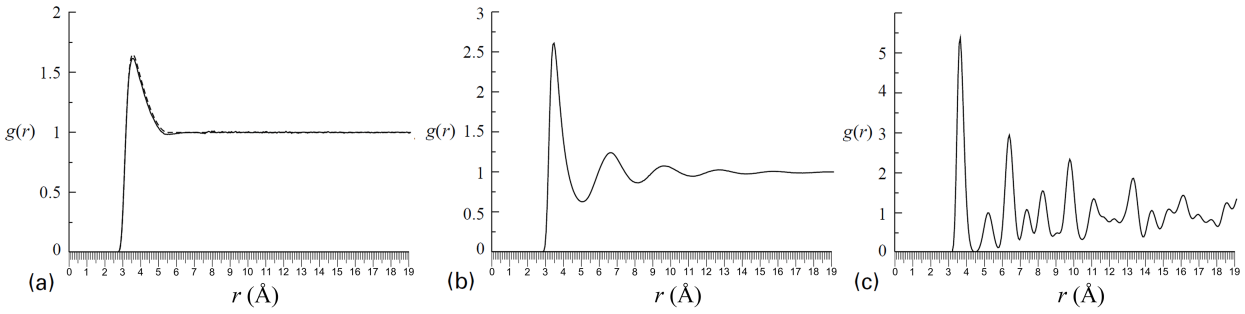

Figure 4: Radial distribution functions for Lennard Jones particles in various states.