Utrecht University
Exam Structure of Matter
Monday, April 18th, 2016
Time: 13:30 - 16:30

Read the questions carefully. Answer the questions in the spaces provided on the question sheets. If you run out of room for an answer, continue on the back of the page.

Name and student number: _____

Good luck!

- Calculators, graphical or otherwise, are not allowed.
- Please note that you can earn a maximum of 83 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:

$$\cos(2a) = 2\cos^2 a - 1$$
$$\cos(a+b) = \cos(a)\cos(b) - \sin(a)\sin(b)$$
$$\cos(a-b) = \cos(a)\cos(b) + \sin(a)\sin(b)$$
$$e^{ik} + e^{-ik} = 2\cos(k)$$

Question 1: **Atomic Physics** ..... *14 points*

(a) (1 point) When going down a group in the periodic table, the size of an atom decreases

A. True

B. False

(b) (1 point) When crossing a period of the periodic table from left to right , the size of atoms increases

A. True

B. False

(c) (3 points) Calculate how many electrons the 'shell' with main quantum number $n = 4$ can accommodate.

(d) (2 points) Give the electron configuration of F ($Z = 9$)

(e) (2 points) Give the electron configuration of Fe ($Z = 26$

(f) (5 points) The electron affinity (E_a) of atom A is defined as the energy difference between the neutral atom and the anion:

$$E_a = E(A) - E(A^-) \tag{1}$$

The electron affinity of an element is determined in a large part by the energy of the lowest empty orbital of the ground state atom. The energy of this orbital is related to the effective nuclear charge of the atom. In which part of the periodic table do you expect to find the atoms with the highest electron affinity? Explain.

Question 2: **Molecular Physics** ..... *26 points*

(a) (1 point) Give the correct order of magnitude of the energy associated with a covalent bond

A. 1 eV
B. 0.1 eV
C. 0.01 eV
D. 0.001 eV

(b) (1 point) Give the correct order of magnitude of the energy associated with an ionic bond

A. 1 eV
B. 0.1 eV
C. 0.01 eV
D. 0.001 eV

(c) (1 point) Give the correct order of magnitude of the energy associated with a van der Waals interaction

A. 1 eV
B. 0.1 eV
C. 0.01 eV
D. 0.001 eV

(d) (1 point) Give the correct order of magnitude of the energy associated with a hydrogen bond

A. 1 eV
B. 0.1 eV
C. 0.01 eV
D. 0.001 eV

(e) (2 points) Which two principles form the basis of tight-binding calculations?

(f) (4 points) Consider the reaction between butadiene (C_4H_6)and an electrophile (HBr), as indicated in Figure 1 below. The electrophile can attack at one of the central carbon atoms *or* at a terminal carbon atom. As indicated in the figure, the product of the reaction depends on where the HBr attacks the butadiene. The rate of a chemical reaction is proportional to the barrier height (ΔE), which is defined as the energy difference between the species with the highest energy (the so-called transition state, structures indicated in the figure) and the reactant (in this case butadiene). The energy of butadiene is $E_{butadiene} = 4\alpha + 4.48\beta$ (**there is no need to calculate this again!**). Recall that both α and β are negative. The energy of a H atom within the Hückel approximation is zero. Assume that there are no changes in the $\sigma-$orbitals.

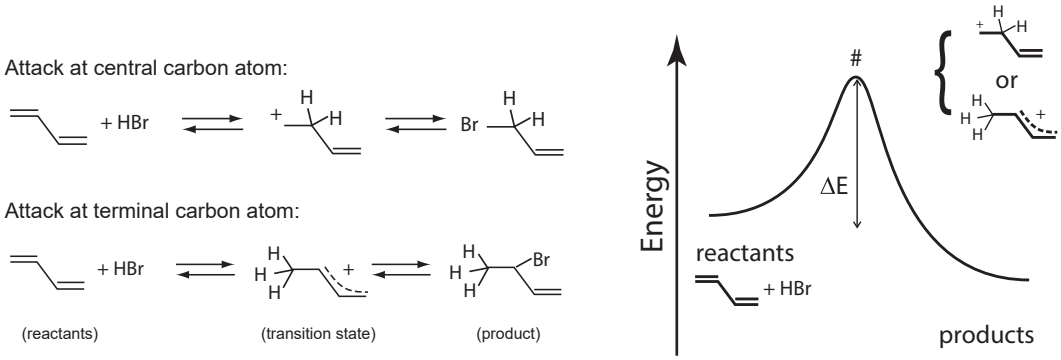

Figure 1: Electrophilic addition reaction of butadiene. Two possible reaction pathways, including the reaction intermediates (transition states) are indicated.

Look at the structure of the transition states. For each transition state, indicate how many carbon atoms are part of the π-conjugated system.

(g) (16 points) Use a Hückel calculation to estimate ΔE (the barrier height) for the two different pathways indicated in Figure 1 **and** state what is the expected dominant product of the chemical reaction. **Hint:** Recall that Hückel calculations are done on π-conjugated molecules.

Question 3: **Condensed Matter Physics 1** ..... *11 points*

(a) (4 points) Consider a two-dimensional crystal (i.e. not a quasicrystal). Which rotational symmetries can the unit cell of such a crystal have?

(b) (2 points) Explain why only the rotational symmetries given under a are allowed.

(c) (1 point) Consider a line of lattice points A-O-B, separated by distance a (indicated in blue). Rotate the entire row by $\theta = +2\pi/n$ and $\theta = -2\pi/n$ (orange and green lines), with point O kept fixed. If the rotation over $\theta = +2\pi/n$ corresponds to a symmetry operation of the lattice, lattice points A is moved to lattice point C . Similarly, rotation over $\theta = -2\pi/n$ maps lattice point B to D.

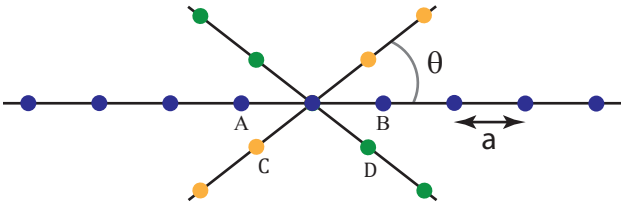

Figure 2: Line of lattice points (blue). Rotations over $\theta = +2\pi/n$ and $\theta = -2\pi/n$ result in orange and green lines, respectively.

Without calculating: what is the distance between **C** and **D** if the rotation corresponds to a symmetry operation of the lattice?

(d) (4 points) Calculate the restrictions this imposes on n.

Question 4: **Condensed Matter Physics 2** ..... *24 points*

Consider a 2D square lattice with a two-atom basis shown in the figure below.

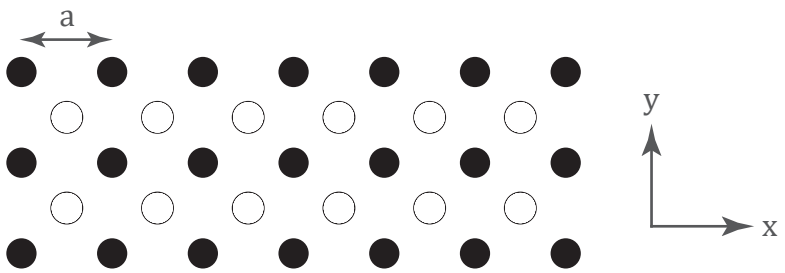

Figure 3: 2D square lattice. Atoms are indicated by black circles.

(a) (4 points) Indicate a unit cell AND the corresponding unit cell vectors in Figure 3.

(b) (4 points) In case each atom contributes one s-orbital that contributes to bonding. The simplest LCAO wave function for this system is given by

$$\psi_t(x) = \frac{1}{\sqrt{N}} \sum_n e^{i\boldsymbol{k}\boldsymbol{R}} \left[c_1 \psi_1(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{\tau}_1) + c_2 \psi_2(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{\tau}_2) \right] \tag{2}$$

Give the meaning of each term/factor in this expression for the wave function.

(c) (1 point) How many electronic bands will you find when you perform a tight-binding calculation with this wave function?

(d) (15 points) Show that the band structure for a square lattice with a two-atomic basis, as calculated using tight-binding, with nearest neighbor interactions only, is given by

$$E(\boldsymbol{k}) = \alpha \pm 4\beta \cos\left(\frac{\boldsymbol{k}\cdot\boldsymbol{a_1}}{2}\right)\cos\left(\frac{\boldsymbol{k}\cdot\boldsymbol{a_2}}{2}\right) \tag{3}$$

Use $\alpha_1 = \alpha_2$

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

(a) (8 points) Structures with a significant degree of disorder are typically described using a radial distribution function, such as shown in Figure 4. Describe the origin of the different features seen in this plot.

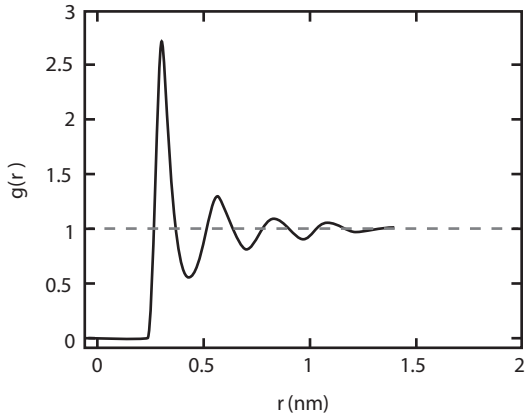

Figure 4: Radial distribution function.