Utrecht University
Solids & Solid Surfaces
Tuesday, January 31st, 2017
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 75 points (which will correspond to a 10.0).
- Not each question is worth the same number of points. Suggestion: save the most difficult/time consuming questions for last.
- The following relations might be helpful:

$$e^{-x} \approx 1 - x \text{ for small } x$$
$$\sin(x) \approx x \text{ for small } x$$
$$\cos(2a) = 2\cos^2 a - 1$$
$$e^{ia} + e^{-ia} = 2\cos(a)$$
$$\cos(\pi/2 + a) = -\sin(a)$$

Question 1: **The Lieb lattice** ..... *21 points*

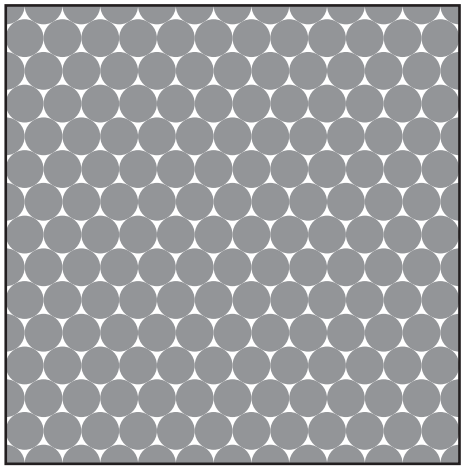

Figure 1: The surface of a particular Cu crystal.

(a) (2 points) Figure 1 shows part of a specific surface of a Cu crystal. Cu has a face-centered-cubic crystal structure. Give the Miller indices of this plane.

(b) (2 points) Indicate the $[1\bar{1}0]$ and $[11\bar{2}]$ directions in the figure.

(c) (1 point) How many equivalent $[1\bar{1}0]$ directions are there in this plane? Explain your answer in the next question.

(d) (3 points) Explain your answer to the previous question.

(e) (2 points) This particular Cu surface exhibits an electronic surface state with an energy close to the Fermi level. What is the physical reason a surface state can exist?

(f) (3 points) Sketch the shape of a surface state wave function along a line from the bulk to the surface to the vacuum above the surface.

The surface state can be thought of as a 2D free electron gas. Picture the surface state electrons as waves. The electrons in the surface state are scattered by adsorbates that are located on top of this surface. If there are multiple adsorbates, one can get constructive- and destructive interference. If there is constructive (destructive) interference, the amplitude of the wave function is enhanced (reduced) locally. An enhanced (reduced) amplitude implies a higher (lower) probability to find an electron at these locations. Hence, by positioning adsorbates with atomic scale accuracy, the surface state electrons can be confined to regions of choice. This opens up the possibility to create lattices of electrons. In class, I showed how the Manoharan group at Stanford used this approach to engineer a honeycomb lattice of electrons.

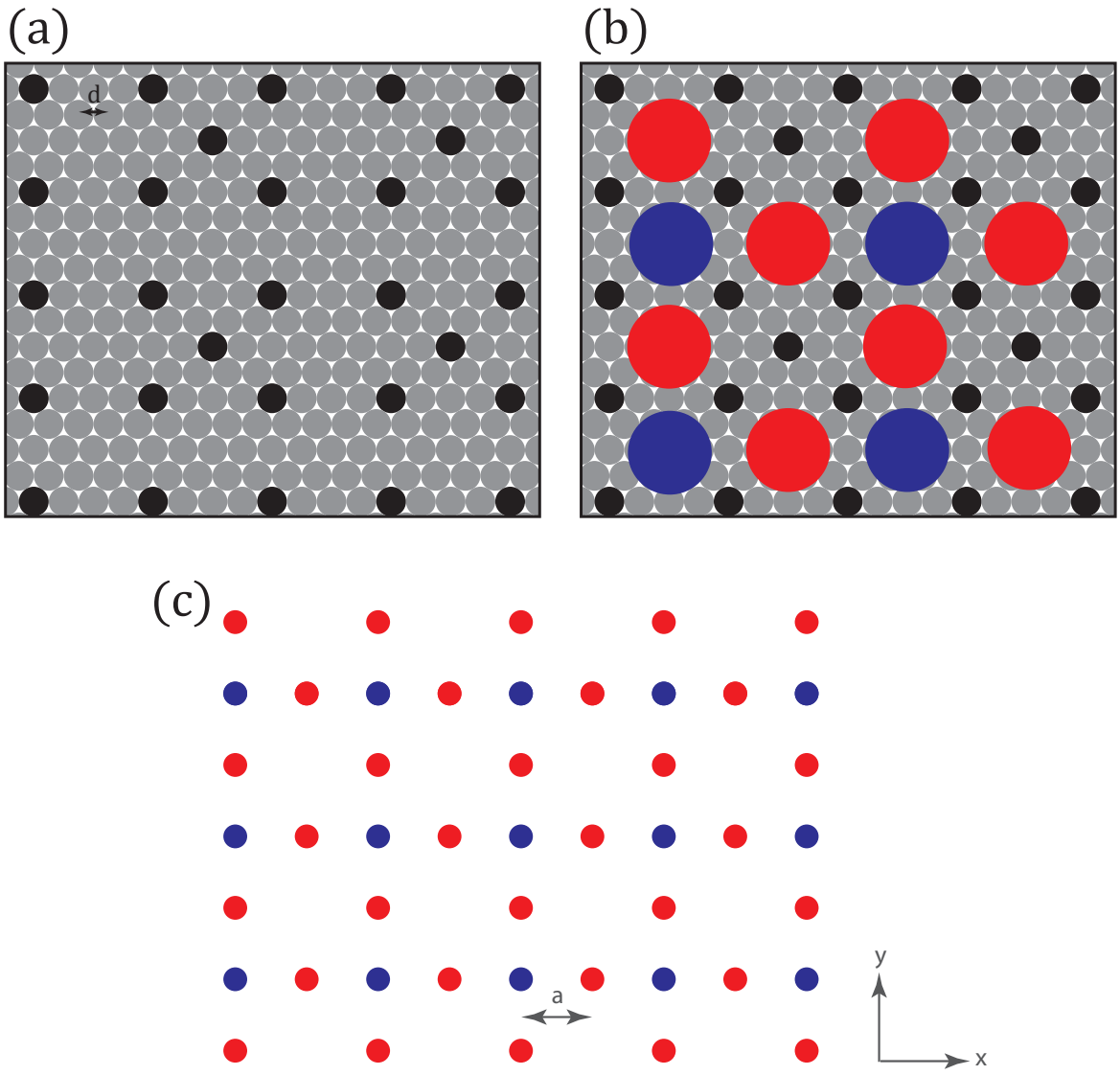

Figure 2: **(a)** CO molecules (black) adsorbed on top of a Cu surface (gray). **(b)** The CO molecules confine the electrons to the regions indicated in blue and red. These are called corner and edge sites respectively. **(c)** Larger piece of the electron lattice with CO molecules and Cu surface omitted for clarity.

(g) (2 points) Consider the arrangement of CO molecules shown in Figure 2a. Indicate the unit cell in Figure 2a.

The CO molecules confine the electrons to the regions shown in Figure 2b. There are two nonequivalent sites: one with 4 neighbors (corner sites, indicated in blue) and one with two neighbors (edge sites, indicated in red). Hence, the arrangement of CO molecules shown in Figure 2a effectively generates the electron configuration shown in Figure 2c. The lattice in Figure 2c is known as the Lieb lattice. Until recently, it was only studied theoretically.

(h) (6 points) Given that the basis vectors in real-space electron lattice are $\boldsymbol{a_1} = (2a, 0)$ and $\boldsymbol{a_2} = (0, 2a)$, determine the basis vectors of the reciprocal space unit cell. **Hint:** $\boldsymbol{a_i} \cdot \boldsymbol{b_j} = 2\pi\delta_{i,j}$.

Question 2: **The electronic structure of the Lieb lattice** ..... *44 points*

In the following, you will perform a tight-binding calculation on the Lieb lattice to investigate its band structure.

(a) (2 points) On which two principles is tight-binding based?

(b) (5 points) Consider the case that each site in the unit cell contributes one s-orbital to bonding. The simplest wave function for this system is given by

$$\psi(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_R e^{i\boldsymbol{k}\boldsymbol{R}} \left[c_1\phi_1(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{\tau}_1) + c_2\phi_2(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{\tau}_2) + c_3\phi_3(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{\tau}_3)\right] \tag{1}$$

Give the meaning of the following terms:

- $\frac{1}{\sqrt{N}}$
- $\sum_R$
- $e^{i\boldsymbol{k}\boldsymbol{R}}$
- c_i
- $\phi_i(\boldsymbol{r} - \boldsymbol{R} - \boldsymbol{\tau}_i)$

(c) (2 points) How many electronic bands will you find from the tight-binding calculation?

(d) (10 points) Show that a tight-binding calculation on the Lieb lattice, taking into account only interactions between nearest neighbors, gives rise to the following matrix equation

$$\begin{pmatrix} \alpha - E(\boldsymbol{k}) & \beta\left(1+e^{i\boldsymbol{k}\boldsymbol{a_2}}\right) & 0 \\ \beta\left(1+e^{-i\boldsymbol{k}\boldsymbol{a_2}}\right) & \alpha - E(\boldsymbol{k}) & \beta\left(1+e^{-i\boldsymbol{k}\boldsymbol{a_1}}\right) \\ 0 & \beta\left(1+e^{i\boldsymbol{k}\boldsymbol{a_1}}\right) & \alpha - E(\boldsymbol{k}) \end{pmatrix} \times \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \qquad (2)$$

(e) (6 points) Show that the matrix equation given in the previous question leads to the following bands.

$$E = \alpha \text{ and } E(\boldsymbol{k})_{\pm} = \alpha \pm 2\beta\sqrt{\cos^2\left(\frac{\boldsymbol{ka_1}}{2}\right) + \cos^2\left(\frac{\boldsymbol{ka_2}}{2}\right)} \tag{3}$$

(f) (4 points) For the solution $E = \alpha$, show that the coefficient $c_2 = 0$.

(g) (3 points) Using the fact that $c_2 = 0$, explain why the band $E = \alpha$ does not depend on $\boldsymbol{k}$, i.e. why the band is flat.

(h) (5 points) We will now focus on the dispersion relation at the corners of the Brillouin zone. One of these is located at $(\pi/2a, \pi/2a)$. Recall that $\boldsymbol{a_1} = (2a, 0)$ and $\boldsymbol{a_2} = (0, 2a)$. Show that the dispersion relation (equation 3) at this point can be approximated as

$$E(\boldsymbol{k}) = \alpha \pm 2\beta a\sqrt{\Delta k_x^2 + \Delta k_y^2} \tag{4}$$

where $\Delta\boldsymbol{k} = (\Delta k_x, \Delta k_y)$ is the deviation from the Brillouin zone boundary, i.e. $\boldsymbol{k} = \left(\frac{\pi}{2a} + \Delta k_x, \frac{\pi}{2a} + \Delta k_y\right)$. We are interested in the dispersion close to the Brillouin zone boundary, i.e. in small values of Δk_x and Δk_y.
Hint: A Taylor expansion is not required.

(i) (3 points) Focusing on the band structure at the corners of the Brillouin zone, do the electrons in the Lieb Lattice have a dispersion relation more like free electrons or more like those in graphene. Explain.

(j) (4 points) Equation 3 gives the energies as a function of wave vector. Figure 3 shows the band structure of the Lieb lattice. Using this graph, sketch the density of states of the Lieb Lattice.

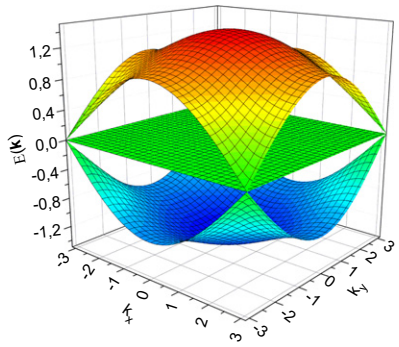

Figure 3: Band structure of the Lieb lattice, including nearest-neighbor interactions only, as given by equation 3.

Question 3: **Characterizing the Lieb lattice** ..... *10 points*

(a) (6 points) A scanning tunneling microscope (STM) can be used to image surfaces with high (often atomic) resolution. Explain how an STM works. The following elements should be included in your explanation: the physical basis of the technique, why you can get high spatial resolution, how an image of the surface is constructed.

(b) (4 points) Sketch the differential conductance spectrum (measured using a scanning tunneling microscope) at a corner site of the Lieb lattice (blue circle in Figure 2, respectively). **Hint:** Use the fact that for the flat band $c_2 = 0$. In addition, you should take equation 4 into account.