Surface Physics - home exam

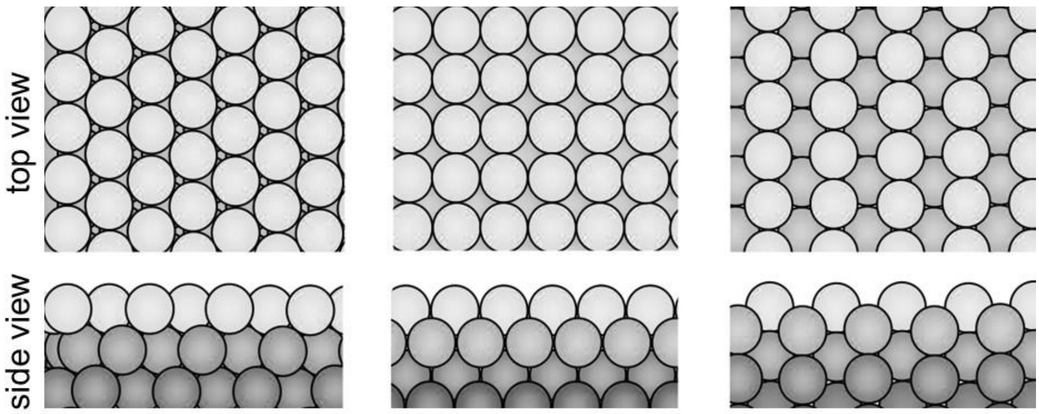
You can freely use any material to answer the questions below. Return the answers (hand-written or typed, but as a single pdf-file) through MyCourses. Copying answers verbatim from literature sources, internet, friends etc. is obviously not ok.

If there are questions, let me know by email (peter.liljeroth@aalto.fi). I will reply to the email and, in addition, post the reply to all the other participants.

There are 6 problems and points for each problem (and sub-problem) are indicated. There are six problems and total maximum for the exam is 46 points.

Problem I (10 points)

The figure below shows three high-symmetry crystal facets of a certain bulk crystal.



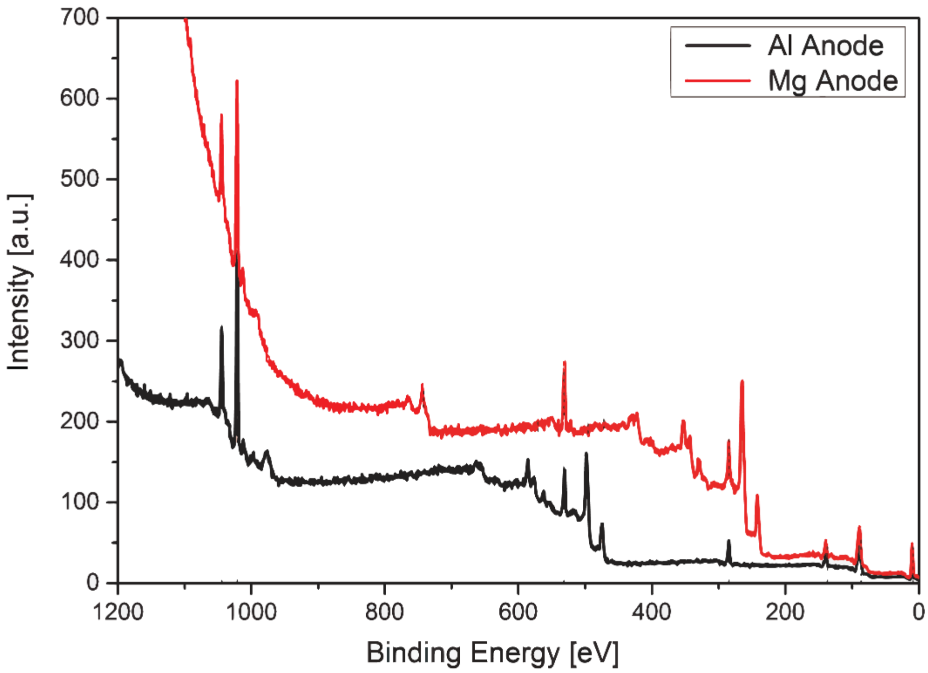
1. Identify the crystal faces and the underlying crystal structure? (2 points)
2. a) Which high-symmetry adsorption sites can be identified on the facet shown on the leftmost panel? (1 point)
   b) How would you estimate the energies of the different adsorption sites within the TSK (terrace-step-kink) -model? (1 point)
   c) Assume that the cohesive energy (and the heat of sublimation) of the crystal is 285 kJ/mol, what would be relative energies of these high-symmetry adsorption sites? (1 point)
   d) What would be the concentration of native adatoms in the most stable adsorption site at temperatures of 300K, 700K, and 1000K? (1 point)
3. a) Draw a sketch of the (1×2) adsorption structure on all these crystal faces. (2 points)
   b) Sketch the corresponding LEED diffraction patterns and indicate the main substrate and overlayer spots. (2 points)

Problem II (6 points)

Write an essay on the “universal curve”. Discuss what is it, what determines the curve and how it is related to surface sensitivity of experimental surface science techniques.

Problem III (10 points)

Below are two photoelectron spectra measured with different x-ray sources: Al Kα radiation at 1486.6 eV (black line) and Mg Kα radiation at 1253.6 eV (red line).

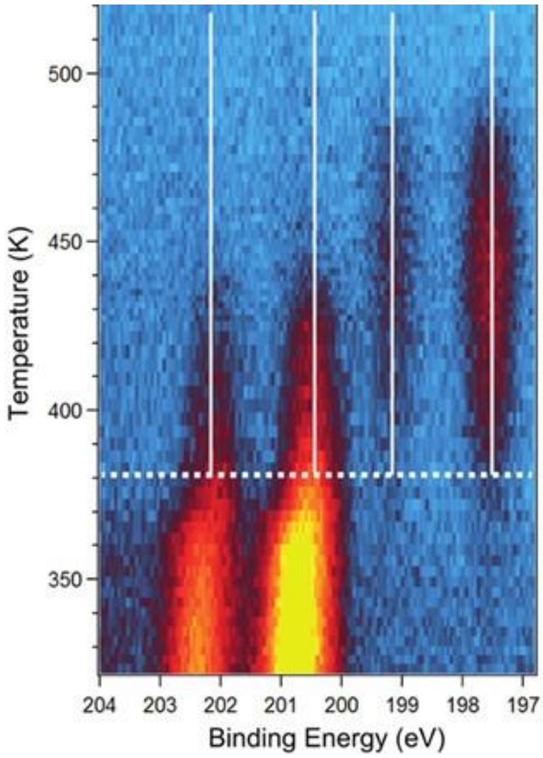


1. What is measured in XPS and how is this converted to the curves shown above? (2 points)
2. Why do some of the peaks shift with different x-ray energies? (2 points)
3. Identify (mark in the spectra) peaks corresponding to photoelectrons. Justify your choice briefly. (2 points)
4. What processes do the other peaks correspond to? Identify the non-photoelectron peaks in the two spectra. (2 points)
5. The energies of the oxygen atomic levels are 532 eV (1s), 24 eV (2s), and 7 eV (2p). Which peaks in the spectra correspond to electrons originating from oxygen? (2 points)

Problem IV (4 points)

The figure below shows high-resolution photoelectron spectrum (yellow: high intensity, blue: zero intensity) measured on the molecules show on the left on a Ag(111) surface as a function of the sample temperature. The spectra show XPS peaks originating from chlorine.

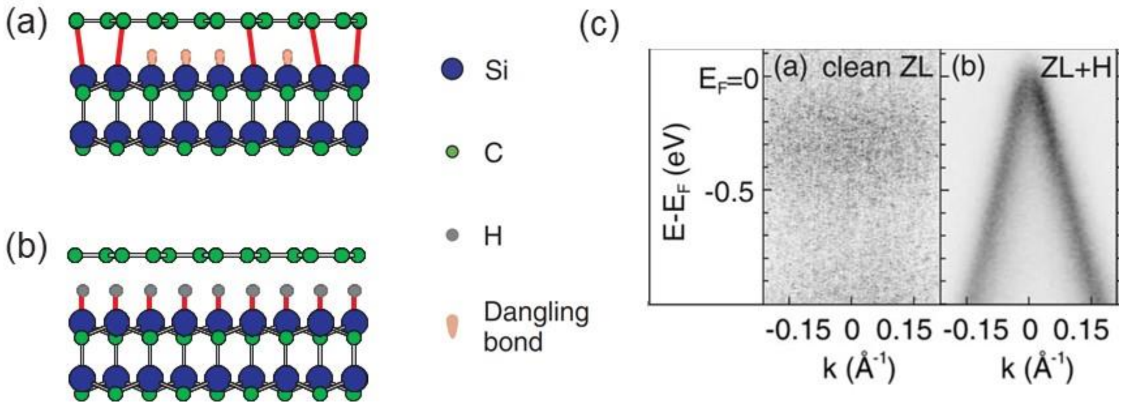
10,10’-dichloro-9,9’-bianthracene



1. Explain the origin of the four peaks: Why are there four different components and why are their energies different? (2 points)
2. What are the processes that happen as the temperature is increased (causing the reduction in the intensity of the two features at higher binding energy and the increase and subsequent reduction in the intensity of the lower binding energy features in the spectra)? (2 points)

Problem V (6 points)

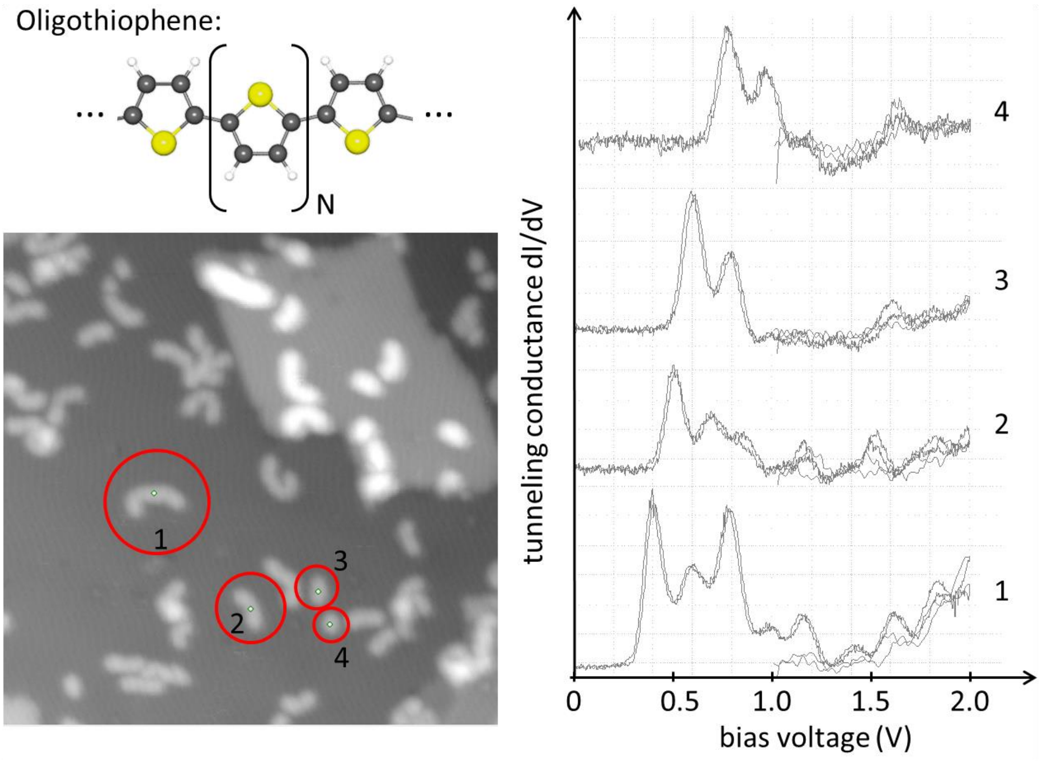
The figure below shows the structure of graphene on silicon carbide substrate (https://en.wikipedia.org/wiki/Epitaxial_graphene_growth_on_silicon_carbide): panel (a) shows the strongly coupled "zero layer (ZL) graphene" and panel (b) shows the graphene decoupled from the substrate via hydrogen intercalation. The panel (c) shows ARPES spectra measured on these systems.



1. What is measured in an ARPES experiment and what sample property can be probed? (2 points)
2. Explain why the ZL graphene shows essentially no features in the ARPES spectrum and why they are there in the ZL+H sample? (2 points)
3. a) Calculate the graphene Fermi velocity from the ARPES measurements and compare it to the expected literature value. (1 point)
   b) What would be the value of the hopping parameter in a nearest-neighbour tight-binding model corresponding to this Fermi velocity? (1 point)

Problem VI (10 points)

The figure below shows the structure of oligothiophene, an STM image with several oligothiophene molecules with different lengths and d*I*/d*V* spectra measured on the four highlighted molecules.



1. How does an STM work and what is displayed in a current feedback image (like above)? What is the signal due to? (4 points)
2. Explain what is measured in the d*I*/d*V* tunneling spectrum and what information can be obtained on general sample? What about in particular on a molecular system. (3 points)
3. Why does the first feature on the d*I*/d*V* spectra shift from molecule to another (molecular lengths from 1 to 4 are 38 Å, 21 Å, 15 Å, 10 Å). Model the system as a particle in a box and estimate the effective mass of electrons in oligothiophene. (2 points)
4. What do the higher bias voltage peaks correspond to? (1 point)