

HOMEWORK ASSIGNMENT # 2

- Describe how the spots in a LEED pattern would evolve if:
 - incident molecules adsorbed randomly onto a surface forming an ordered overlayer only when one quarter of the substrate atoms are covered;
 - an overlayer is ordered in one direction but not in the orthogonal direction.
- For structures b,c,h in Figure 2.29, determine the LEED patterns. Classify the adsorbate (black) structures in matrix notation. Calculate the coverage (fraction of a monolayer).
- For the LEED patterns a,c,g,i in Figure 2.30, determine the surface structures. Substrate reflexes are marked with dark circles while additional adsorbate reflexes are marked with x's. The substrates are supposed to be fcc(100) (a-c) and fcc(111) (g-i). Also, draw the adsorbates over the substrate atoms (coordination number = 1).
- Motivate the tunneling equation for STM. Hint: look up a quantum book on 1-D tunneling.
- In an STM image, does an adsorbate sitting on top of a surface always look like a raised bump compared with the substrate?
- Some adsorbates can be imaged in STM at low temperatures but seem to disappear at higher temperatures even though they have not desorbed from the surface. Explain.
- The dimer unit on a Si (1 0 0) surface has a bonding orbital just below E_F and an antibonding orbital just above E_F . Make a prediction about STM images that are taken at positive compared with negative voltages. Do the images look the same and, if not, how do they differ?
- Consider the spectrum of adsorbed CO shown in Figure 2.24. CO is adsorbed as part of a Rhodium-containing molecule (see Figure 2.31) on an Al_2O_3 substrate. Explain why there are two peaks and not just one, and explain why the positions of the peaks change when ^{18}O is used.
- Draw qualitative pictures of the photoelectron spectra of clean transition metals in which the 3d orbital is partially filled and overlaps with the lower 4s orbital. The 3d band is narrower and has a higher density of states.

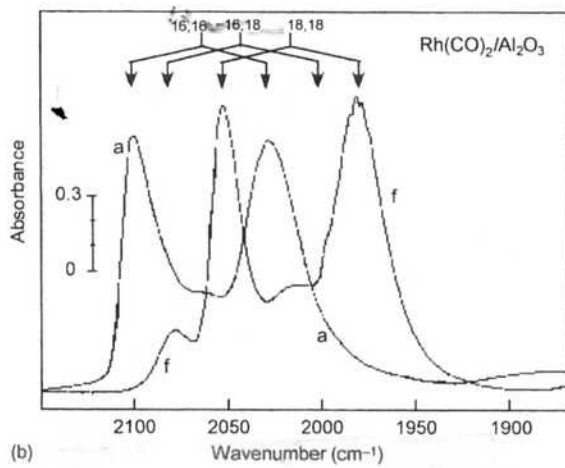


Figure 2.24 The infrared spectrum of (a) gas-phase CO compared with that of (b) CO adsorbed on

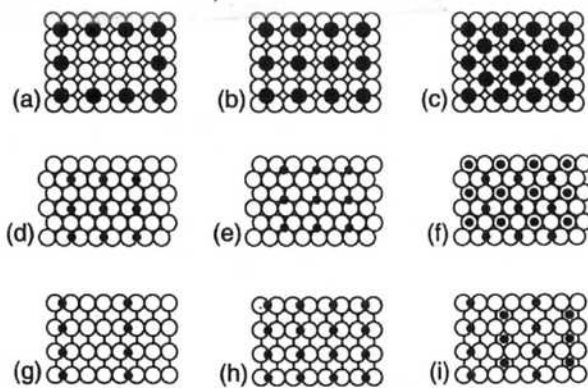


Figure 2.29 Structures (a)–(i): see Exercise 2.8

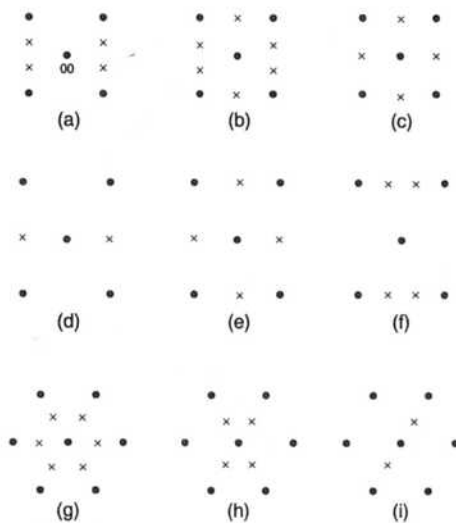


Figure 2.30 Low-energy electron diffraction (LEED) patterns (a)–(i): see Exercise 2.10

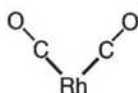


Figure 2.31 CO adsorbed as a gem-dicarbonyl on rhodium atoms present on an Al_2O_3 substrate (substrate not shown): see Exercise 2.13