

**Physics 243A - Surface Physics of Materials**  
**Midterm Examination**  
**November 13, 2008**  
(100 points total, open books, notes, and class handouts)

Name: \_\_\_\_\_

[1] (15 points) Suppose that the sticking probability for oxygen molecules ( $O_2$ ) incident on a W(110) surface at 298 K and an ambient pressure of  $1 \times 10^{-8}$  torr is constant at 1.0 until a coverage of atomic oxygen of 0.5 monolayers (as measured relative to the W atom surface density of  $1.41 \times 10^{15}$  atoms/cm<sup>2</sup>) is reached. Above this coverage, assume that the sticking probability drops to 0.1. Calculate the time variation of the coverage of atomic oxygen on the surface, make a qualitative plot of coverage versus time, and determine how long it will take to reach a full coverage of 1.0 monolayer.

[2] (25 points) A Hartree-Fock calculation for the CO molecule yields a total energy for the system of -112.75 atomic units (1 a.u. = 27.211 eV) and one-electron eigenvalues  $\epsilon_{C1s} = -20.65$  a.u. and  $\epsilon_{O1s} = -11.30$  a.u. The distance between C and O in the calculation was set to be the equilibrium distance of 1.18 Å.

- (a) Estimate the O 1s and C 1s binding energies in eV from this data.
- (b) What additional theoretical total energies would you need to be able to calculate the relaxation energies involved with the O1s and C 1s binding energies? Specify these as precisely as you can.
- (c) After photoelectron ejection from the C 1s orbital, what *other* molecule's outer electron orbitals would best represent the final outer electron orbitals of the resulting ion?
- (d) Write down the equations for the coulomb and exchange integrals between the C 1s and O 1 s orbitals. Then provide numerical estimates for *both* of these integrals, using a simple classical model if appropriate. Note that these two core orbitals are on two different centers and so overlap negligibly. Also, it may be convenient to note that two classical electron point charges separated by a distance of 1 Å have a repulsive potential of 14.4 eV.

[3] (20 points) Consider KLL Auger emission from Cu metal, with some relevant binding energies being:

Cu:	Z = 29	Zn: Z = 30
M4,5	??	10.2
M3	75.1	88.6
M2	77.3	91.4
M1	122.5	139.8
L3	932.5	1021.8
L2	952.3	1044.9
L1	1096.7	1193.6
K1	8980.5	9660.8

- (a) What will be the most energetic Auger electron in this series? Make the most accurate estimate you can of its energy, indicating the type of formula you have used.
- (b) After the Auger transition in (a), what type of hole state will be left behind? If we now want to estimate the effect of this hole state on the surrounding valence electrons, we might treat the final state as an "impurity atom" in the Cu lattice. What would be the atomic number of the atom we would choose for the impurity in this case?

(c) From what we have said about the band structure of Cu metal in lecture, can you estimate the binding energy of the M4,5 levels above, as judged relative to the Fermi level? Explain your answer.

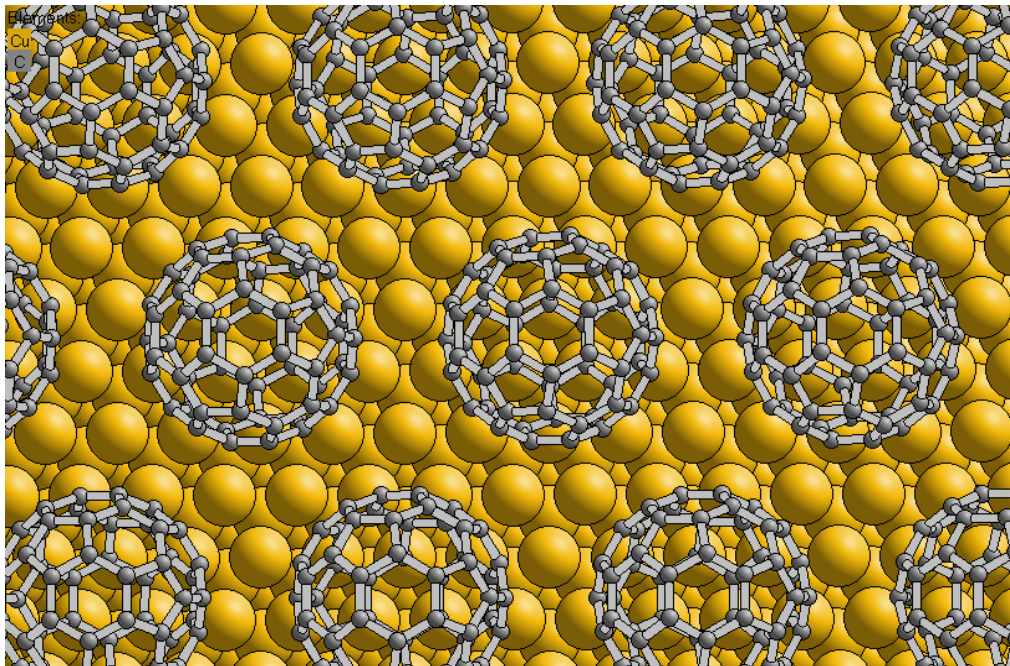
(d) What will be the energy of the Cu  $K\alpha_1$  x-ray?

[4] (40 points) This problem consists of several independent parts. Answer each part briefly.

(a) (10 points) If a bulk alloy of 40% Ru and 60% Mo were prepared, would the composition of an atomically clean surface of this alloy be expected to be different from that in the bulk? Why or why not?

(b) (15 points) Consider an idealized two-dimensional material whose "surfaces" are the one-dimensional lines or curves describing its boundaries. Assume that the material has a simple cubic crystal structure and that the "surface tension", now in units of energy/length, is smallest along  $\langle 100 \rangle$  type directions parallel to the cube directions, where it has a normalized value of 1.00. The surface tension is next smallest along  $\langle 110 \rangle$  directions at  $45^\circ$  with respect to  $\langle 100 \rangle$ , where it has a value of 1.25, and it is much larger along any other direction. From this information, use the Wulff construction to predict the shape of a sample of this material at equilibrium, including in particular, the fraction of surface of  $\{100\}$  type and the fraction of  $\{110\}$  type.

(c) (15 points) The stereographic image below shows the structure of  $C_{60}$  "buckyballs" adsorbed on a Cu(111) surface.



(i) What would you call this structure in Wood notation, treating the  $C_{60}$  molecules as a single unit?

(ii) What would the LEED pattern qualitatively look like for this surface, considering only the strongest spots from the top Cu layer and the  $C_{60}$ ? Indicate clearly which spots come from the Cu, the  $C_{60}$ , and from both of them.

(iii) If the  $C_{60}$  array were translated by  $2.0 \text{ \AA}$  to the right, would your answer to part (ii) change? Explain why or why not.