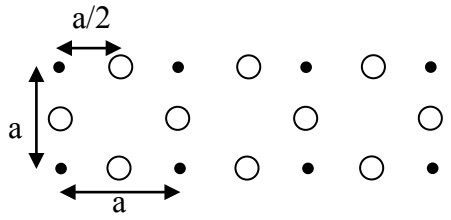
Long problem 2

Show all your calculations. Write in pen, not in pencil, otherwise I can't read it.



A piece of a two-dimensional infinite lattice is shown in the picture above.
The dark circles are Cu atoms, the open circles are O atoms.
Consider the tight binding band structure that results from the orbitals $d_{x^2-y^2}$ on the Cu atoms and the p_x or p_y O orbitals that point along the Cu-O bond. I.e. a single orbital per atom. Assume they are all orthogonal to each other.
Assume the only non-zero matrix elements of the electronic Hamiltonian in this basis are the diagonal ones, the one involving nearest neighbor Cu and O atoms, and the one involving nearest neighbor O atoms. Call them ε_d, ε_p, t_d, t_p for: diagonal for Cu and O, off-diagonal for Cu-O and O-O respectively.

(a) What is the sign of t_d and t_p?

(b) Construct the Hamiltonian matrix $H_{nn'}(\vec{k})$

(c) Find all the energy eigenvalues at the $\vec{k}$-points $\Gamma = (0,0)$, $X = (\pi/a, \pi/a)$, and $D = (\pi/a, 0)$ in terms of the Hamiltonian matrix elements.

(d) Assume the lowest and highest energy eigenvalues at points Γ and X have values -3.5ev and -2eV at point Γ, and values -6.6eV and +3.6eV at X. Assume also that $\varepsilon_p < \varepsilon_d$ and that both the lowest and highest energy eigenvalues at X depend on the value of t_d. Using this information, find numerical values for the Hamiltonian matrix elements ε_d, ε_p, t_d, t_p in eV.

(e) List the values of all the energy eigenvalues at points Γ, X and D, in eV.

(f) Make a plot of the band structure along the lines $\Gamma - X - D - \Gamma$ using the numerical values found for the Hamiltonian parameters.

(g) Assuming the Fermi energy is $\varepsilon_F = 0$ and the lattice constant is $a = 2.5A$, find the electron density n in units electrons/cm^3.

(h) For extra credit: calculate the electronic density of states $g(\varepsilon)$ and make a plot of it versus ε.

Useful reference: Slater and Koster, Phys. Rev. 94, 1498 (1954).