MS 131, Problem Set #6

revised 11/11/05
due 11/16/05

1. Using the LCAO model for insulating solids (where insulators means all non-metallic solids) compare the effective mass of more ionic compounds from those that are more covalent.
2. Consider the Kronig-Penney model for a 1-dimensional solid with a periodic potential, where the height and width of the barrier are arbitrary. Using the requirements that the wave function and its first derivative be single-valued and continuous, derive four equations that place restrictions on the allowed values of k, α, and β, and therefore E.
3. The Kronig-Penney model of 1-dimensional solids (under the approximation of periodic energy barriers that are delta functions) requires that k be restricted to values that makes the following relationship true

$$\mu\left(\frac{\sin \alpha a}{\alpha a}\right) + \cos \alpha a = \cos ka$$

where μ is the barrier strength, a is the interatomic distance and α is related to energy.

(a) Plot the left hand side of this relationship as a function of αa for an arbitrary value of μ and indicate the regions of forbidden values of k. Explain why these are forbidden.

(b) Determine the width of the first energy gap predicted by this model in terms of μ and a. In order to obtain an analytical answer, expand sin(x) and cos(x) to their algebraic forms, using terms no higher than x^2.

4. Consider a two-dimensional solid comprised of A atoms distributed on a square lattice. The lattice constant is a. The Bloch sum wave function is:

$$\psi_{\vec{k}}(\vec{r}_{p,q}) = \sum_{n=1}^{N} e^{i\vec{k}\bullet\vec{r}_{p,q}} \chi_{p,q}(r) = \sum_{n=1}^{N} e^{i(k_x pa + k_y qa)} \chi_{p,q}(r)$$

(a) Plot the phases at the atoms [the value of $\cos(\boldsymbol{k}\cdot\boldsymbol{r}_{p,q})$] for $\boldsymbol{k}$ = (0, 0), (π/a, 0), (0, π/a) and (π/a, π/a).

(b) Plot energy as a function of k_x, k_y in the form of a contour plot over the first Brillioun zone, ($-\pi/a$, $-\pi/a$) to (π/a, π/a), for the s orbitals. Indicate the value of E(k) at (0, 0), (π/a, 0), and (π/a, π/a)

(c) Plot E(k) in a standard x-y plot, where k follows the triangular path from (0,0) = Γ, to (π/a, 0) = X, to (π/a, π/a) = M, and back to (0,0) = Γ.

(d) Make a sketch of p_x and p_y orbitals (with the phases on the lobes indicated) for $\boldsymbol{k}$ = (0, 0), (π/a, 0), (0, π/a) and (π/a, π/a). Indicate the kind of bonding or anti-bonding that these states represent (σ and/or π). Rank the energies for these states.