

Assignment 7

Due: Friday, Nov. 2 at 4 pm

Reading: Livingston 10.1-10.4, 11.1-11.2, 11.5-11.6

Assigned exercises (group problems unless otherwise noted):

Livingston:

10-2 (You are meant to ignore the inter-electron repulsion; this is a reasonable approximation, since the electrons can move about quickly, and tend to stay away from one another.)

10-3 (Don't expect good agreement with experiment for part c, though it should be within an order of magnitude.)

10-5

10-9

11-9

7A. Shown here is the energy vs. k_z graph for the simple cubic lattice in the tight-binding, Hückel approximation, for the line through k -space with $k_x = k_y = \frac{\pi}{2a}$. The horizontal axis does not necessarily

correspond to $\langle \epsilon \rangle = 0$; in fact the $\langle \epsilon \rangle = 0$ level would likely be considerably higher given the vertical scale used for this figure. You'll recognize the lower band as the one we discussed in class, that arises from an s AO. Assume it arises from the 2s orbital. The upper band shown arises from the 2p_z orbital. (I assume you are familiar with p orbitals. However, you might want to look at Livingston's figure 9.4 on p. 159 just to remind yourself.) Because the probability density for a p orbital is focused along a particular axis, it extends further along that axis than the s orbital does. For the upper (2p) band shown in the figure, explain why

- The midpoint of the band is higher than for the band derived from the 2s orbitals.
- The amplitude of the band is inverted compared to the band derived from the 2s orbitals.
- The amplitude of the band is larger in magnitude than that of the derived from the 2s orbitals.

