

MATRL 218: Assignment 4

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1. Sketch the π molecular orbitals formed by the p_z orbitals on each carbon in the benzene molecule. Remember that the ordering of energy levels (going up from most bonding to most antibonding) is 1, 2, 2, 1.
2. Sketch the E vs. k dispersion relation for a square lattice of p_x and p_y orbitals, and pay attention to σ and π interactions. The points defining the Brillouin zone boundaries are $\Gamma(0, 0)$, $X(\pi/a, 0)$, $Y(0, \pi/a)$, and $M(\pi/a, \pi/a)$. Sketch the densities of state alongside. Note that a single band could be σ or σ^* -like in some parts of the Brillouin zone, and π or π^* -like in others, and label these.
3. Now stretch the above the lattice in the y direction so that it is rectangular, with $a < b$. How does this modify the band structure. Remember that the BZ boundaries are $\Gamma(0, 0)$, $X(\pi/a, 0)$, $Y(0, \pi/b)$, and $M(\pi/a, \pi/b)$.
4. Explain how you would use a *local* bonding picture to sketch the density of states of Si (filled valence band and empty conduction band) by recognizing that with 4 electrons per Si and 4 bonds going out of every Si, the compound is electron precise.
5. Can you extend this analysis to amorphous Si?
6. How should one think of the electronic structure of SiO_2 , which has an enormous band gap? Remember that you need to think of the separation between the centers of states that form the valence and conduction band (that can usually be attributed to electronegativity differences) *and* you need to think of the width of the VB and CB (which arises from dispersion — the orbitals involved and the nature of the structure).
7. CaF_2 has an even larger band gap than SiO_2 , which is of great consequence in high-end camera lenses (larger band gaps mean reduced chromatic aberration). Suggest using ideas of electronegativity and band width, why this might be so.
8. I-III-VI semiconductors such as CuInSe_2 , II-VI semiconductors such as CdSe , and III-V semiconductors such as GaAs all have the same rules of electron precision as Si in the diamond structure. Explain these.