MATRL 218: Assignment 5

Ram Seshadri (seshadri@mrl.ucsb.edu)

1. The one dimensional chain compound K_2PtBr_4 has square planes of $PtBr_4^{2-}$ forming chains that are linked through Pt–Pt bonds. Describe the crystal field splitting, and sketch schematic density of states. What does the dispersion along the Pt–Pt bonds look like and which orbital is involved? Is K_2PtBr_4 a metal? How can it be made into a metal.

2. FeS_2 ("fool's gold") has the pyrite structure (octahedral Fe) and because of a bond between the two S atoms (characterized by a short S–S distance), it can be formulated $Fe^{2+}[S_2]^{2-}$. Magnetic measurements suggest that the compound is non-magnetic.

   (a) Sketch out the crystal field (showing t_{2g} and e_g levels) and fill them with the correct number of electrons.

   (b) Sketch out schematic densities of states showing Fe d states and S p states. Do you expect a metal or an insulator?

   (c) What do you expect the situation in CoS_2 to be? It has the same crystal structure.

3. 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.

4. 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 $M(\pi/a,\pi/b)$. Show that if there is one electron per orbital, such a distortion can result in a gap between filled and unfilled states.