MATRL 218/CHEM277: Assignment 5

Ram Seshadri (seshadri@mrl.ucsb.edu)

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1. The one dimensional chain compound K$_2$PtBr$_4$ 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 (and remember we sketched the schematic DOS for PdO). What does the dispersion along the Pt–Pt bonds look like and which orbital is involved? Is K$_2$PtBr$_4$ a metal?

2. Sketch the most bonding and the most antibonding crystal orbitals formed from $sp^2$ orbitals on carbon in graphite. Do the same for $p_z$ orbitals.

3. Sketch the most antibonding $sp^3$ crystal orbital for (a few) Si atoms within the unit cell of diamond Si. Why is molten Si metallic, while crystalline Si is insulating.

4. FeS$_2$ (fools 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.

5. What does the concept of the divergence of susceptibility mean to you. When does the susceptibility diverge for a Curie paramagnet. Explain what happens when (i) ferromagnetic interactions are present, and (ii) antiferromagnetic interactions are present, using the concept of an internal field. Make sketches for all cases.

6. Sketch the magnetic densities of state for antiferromagnetic LaCrO$_3$ (perovskite), and ferromagnetic CrO$_2$ (rutile).