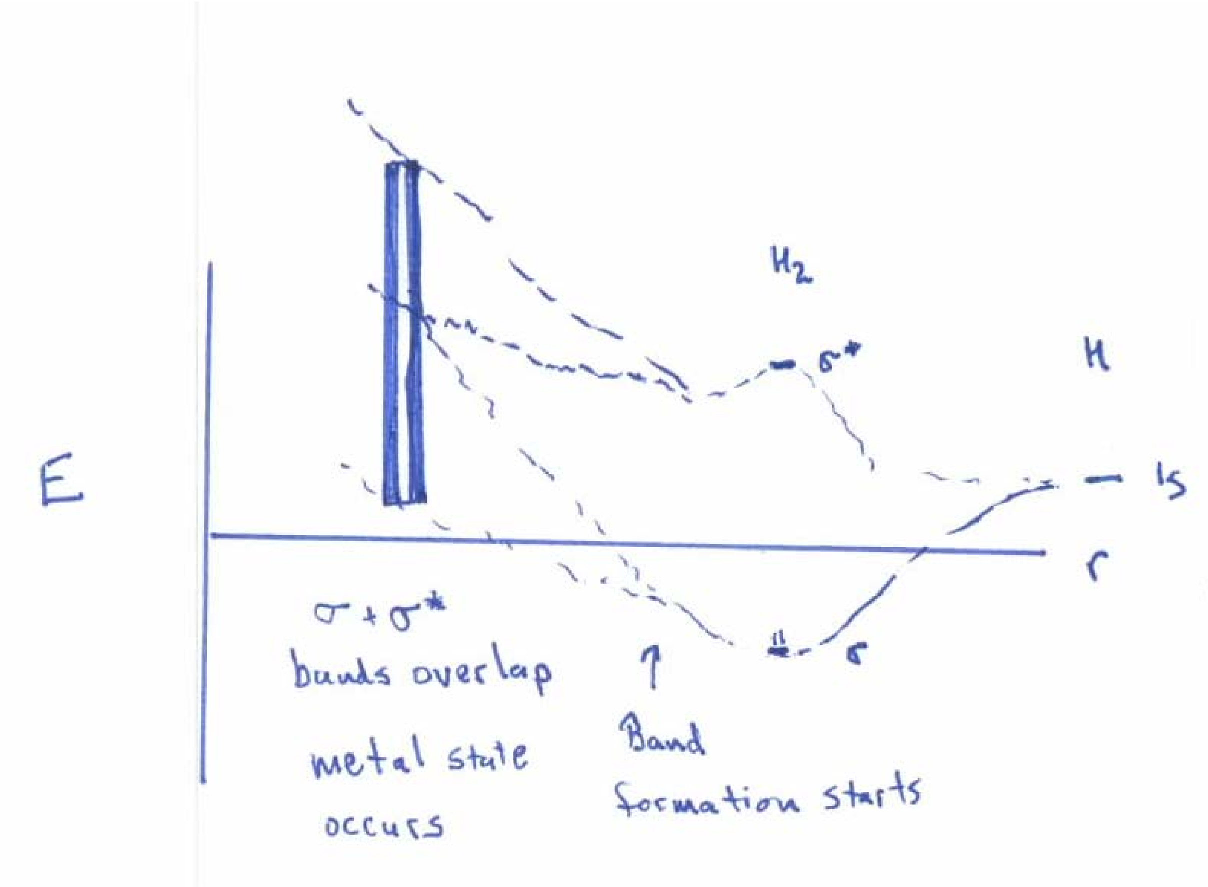
CHM 501
Exam 2
April 6, 2016

1. (15 pts) In class we discussed the nonstoichiometry in Fe_xO. The distribution of Fe^{2+} and Fe^{3+} was wrong in class. Provide the correct stoichiometry for each oxidation state. Is this a p-type or n-type semiconductor?

   Let y and z be the stoichiometry for Fe^{2+} and Fe^{3+}, respectively. Then, y + z = x (to match the total Fe stoichiometry) and 2y + 3z = 2 (to maintain charge balance). Then z = 2 – 2x and y = 3x – 2, so the compound is better represented by $(Fe^{2+})_{3x-2}(Fe^{3+})_{2-2x}O$. There is an excess of Fe^{3+}, which provides positive charge carriers, so this is a p-type semiconductor.

2. (25 pts) It is postulated that on Jupiter the high pressure in the atmosphere is sufficient to cause H_2 to become a metal, and this accounts for the high reflectivity of the planet. Draw an energy diagram as a function of internuclear distance that could explain this prediction.



   At large distances the H atoms are well separated and all of the orbitals are the same energy, that of the H 1s orbital. As the H atoms get closer the dimer H_2 forms, which is quite stable and in an energy well. At higher pressures the H_2 molecules start to get close to each other and the σ and σ* orbitals overlap to form energy bands, with the lower band filled and the upper band empty. At high enough pressure the bandwidths become large enough so that the two bands overlap and the net band is half-filled, which meets the criterion for a metal.

3. (25 pts) The compound CsAu was first reported more than 70 years ago but interest in the compound has recently been renewed. Would you expect this compound to be ionic or a metal alloy? Explain your reasoning.

What experiments might help determine the better bonding description? Explain how to interpret the experiment or experiments you suggest.

Cs is the most electropositive element (except for the radioactive Fr) and Au has a $d^{10}s^1$ electron configuration, making it similar in some respects to the p-block elements, so it has a reasonably large electronegativity. Thus, CsAu is ionic, Cs^+Au^-. A temperature dependent electrical conductivity measurement could support this hypothesis: the ionic compound would have relatively low conductivity at room temperature and this would increase slowly as the temperature was raised and then jump up considerably at the melting point. If the compound were a metal the room temperature conductivity would likely be higher and would decrease as the temperature were raised.

4. (20 pts) Predict the order of melting points of the following compounds: Al_2O_3, NaCl, $CH_3CH_2CH_2CH_3$, CH_3CH_2OH, $CH_3CH_2OCH_3$. Explain your reasoning.

Al_2O_3	>	NaCl	>>	CH_3CH_2OH	>	$CH_3CH_2OCH_3$	>	$CH_3CH_2CH_2CH_3$
Ionic, large E_{lat}		Smaller E_{lat}		H-bonding		dipole-dipole attractions		van der Waal’s

5. (15 pts) An LED that emits red light can be formed with GaAs. What color emission would you expect from a GaN LED? Explain.

The band gap in GaN is predicted to be larger than that in GaAs because the valence orbitals in N are smaller than those in As (2s2p vs 4s4p). The smaller orbitals do not overlap as well so the bandwidths are smaller in GaN and the band gap is larger, which should lead to a higher energy, shorter wavelength emission, in the blue region of the spectrum.