## Home work for March 23 lecture 9 due March 30

- 1. What is the Hund's rule U eff for Gd3+ (4f7) and Eu3+(4f6)
- Lets assume that F0 is reduced to zero in the solid lets also neglect the 3d band width. What then would the energy be of a charge disproportionated lattice in which two Mn3+(d4) ions convert to one each of Mn2+(d5) and Mn4+(d3) i.e. looks like a charge density wave material with an amplitude of 2 electrons.
- 3. Determine the energy level diagram for Ti3+ in octahedral coordination assuming a very large crystal field splitting into t2g and eg and including the spin orbit coupling of the single d electron. Note the lifting of the 3 fold degeneracy and the appearance of an orbital angular momentum.
- 4. Determine the relation for the superexchange interaction between a singly occupied dxz orbital and a singly occupied d(x2-y2) on opposite sides of an O2- ion. Take the 3 atoms to be on a straight line along the x direction. Take into account the on site coulomb interactions and the Hunds' rule coupling for all the states involved. and the charge transfer energy i.e. the energy to excite an O 2p electron to one of the singly occupied d sites.
- 5. Using perturbation theory and hybridization between the TM 3d orbitals and intervening O 2p orbitals determine the splitting of the t2g and eg orbital energies as a result of a tetragonal distortion either a compression or an expansion along the z axis. Take the sigma pd hoping integral to be 2 times that of the pi hoping integral and assume an exponential dependence of the hopping integral on the interatomic distance.