Magnetism in materials

Exercise - Week 03

1. Let's assume that we have a 3d metal in a thetrahedral crystal.

   (a) Between the e_g orbitals and the t_{2g} orbitals, which one would have the highest energy due to the crystal field effect ?

   (b) Find the spin number S for all the 3d metal ($3d^0$ to $3d^{10}$) in the high spin and low spin case.

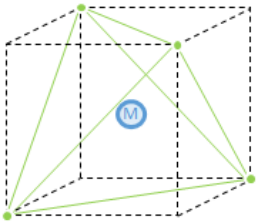

Figure 1: Thetrahedral crystal

2. Using the spin distribution for a octahedral crystal discussed in course (for a 3d metal), determine in which situation the geometry will change due to the Jahn-Teller effect.

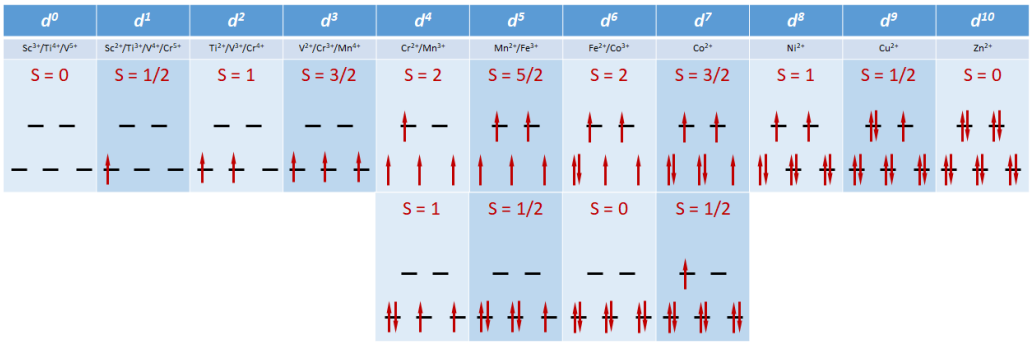

Figure 2: Spin repartition for 3d metal in an octahedral crystal

3. A Sc^{2+} ion has one electron in the 3d shell. It is in an anisotropic crystal and the crystal field can be written as a potential acting on the 3d electron as $E = AL_z^2$. What are the lowest orbital states of the SC ion if $A > 0$ and $A < 0$?
   The spin-orbit coupling λIS is much smaller than the crystal field. When this is included, what are the approximate ground states of the ion, for $A > 0$ and $A < 0$?

4. Vesta is a software used to visualized crystal structure. We will in this exercise use it to analyse Ca3Co2O6 crystal. Download link, file and articles are all on moodle :

   (a) Download and install Vesta.

(b) Load the structure of Ca3Co2O6.

(c) Determine the environment of Co ions and discuss possible arrangements of d-orbital.

(d) Compare the results obtained by measurements of susceptibility, magnetization and neutron diffraction.[1][2]

5. Let us consider a compound ML_6 where six ligands (L) occupy the vertices of an octahedron, and the metal ion (M) resides at the center. We establish a global right-handed coordinate system aligned with the diagonals of the tetrahedron.

   One of the normal modes of vibration associated with ML_6 is the *symmetric stretching*, depicted in (a) where ligands move along the green arrows. The normal coordinate for this mode is given by:

$$Q_1 = \frac{1}{\sqrt{6}}(X_2 - X_5 + Y_3 - Y_6 + Z_1 - Z_4)$$

   where (X_i, Y_i, Z_i) represent deviations of the ligands from their equilibrium positions. Q_1 equals zero when all ligands are in equilibrium, Q_1 is positive when ligands move outward, and negative when ligands move inward.

   In (b) and (c), two additional normal modes termed *asymmetric stretching* are depicted. The green arrows illustrate ligand motion for these modes. Find the normal coordinates for them.

   Note: Generally, electronic states can couple to multiple normal modes or their linear combinations. To visualize this phenomenon, we can utilize the data and simulations provided in the file `Jahn_Teller.ipynb`. Specifically, we aim to depict the Mexican hat energy surface depicting the coupling between electronic states and the vibrational modes Q_2 and Q_3, as introduced in the previous exercise, in the case of linear Jahn–Teller effect within the harmonic approximation.

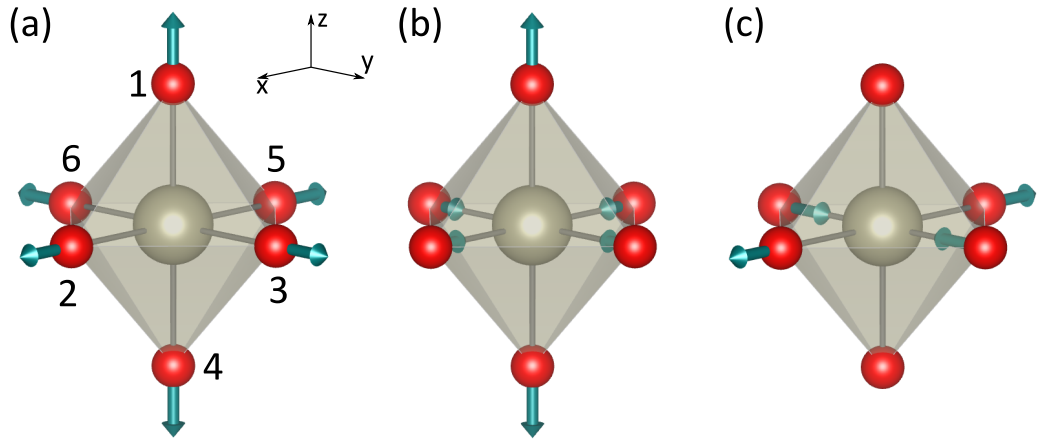

Figure 3: Normal modes of atoms in an octahedral complex ML_6.

References

[1] A. Maignan, C. Michel, A. C. Masset, C. Martin, and B. Raveau. Single crystal study of the one dimensional $ca_3co_2o_6$ compound: five stable configurations for the ising triangular lattice. *The European Physical Journal B - Condensed Matter and Complex Systems*, 15(4):657–663, Jun 2000.

[2] B. Haubackb S. Aasland, H. Fjellvag. Magnetic properties of the one-dimensional $ca_3co_2o_6$. *Solid State Communications*, 101(3):187–192, 1997.