Applications of Group Theory

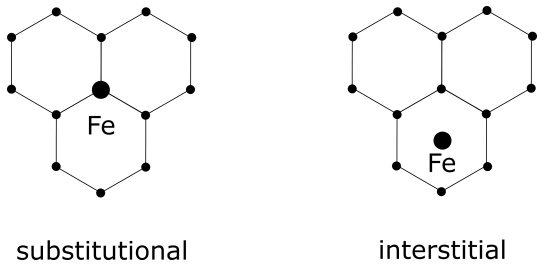
Lectures	Tue	10:00 - 11:30	PHY 9.1.09
	Thu	10:00 - 11:30	PHY 9.1.09
Exercises	Fri	10:00 - 11:30	PHY 5.0.21

Sheet 8

1. Crystal field on an iron impurity

Suppose that an iron (Fe) impurity is introduced into a two-dimensional honeycomb lattice of an insulating host material (see figure).

1. Discuss why the charge on the honeycomb lattice cannot be uniform, if the two-dimensional material is an insulator, but rather have equal value but opposite sign in the two inequivalent atomic position in the unit cell.
2. Write the expression of the crystal field for the impurity both in the interstitial and substitutional positions (see figure below).
3. Find the point symmetry group for the substitutional and interstitial impurity. For the interstitial case, express the results of point 2) in terms of spherical harmonics. In particular, find the strongest non uniform contribution.
4. Calculate crystal field splitting of the fivefold d-levels of the Fe impurity in the crystal fields for the two locations introduced in 2).
5. Identify the basis functions associated with each of the levels considered in 4) and estimate the energetic order of the levels.
6. Indicate how the ordering of the levels might indicate whether the Fe impurity is located substitutionally or interstitially in the honeycomb lattice.



2. Non-splitting crystal field

Show (by finding the characters of the rotation group) that the d-level for a transition metal impurity in a metal cluster with I_h point symmetry is not split by the icosahedral crystal field.

Frohes Schaffen!