University of Regensburg Summer Term 2013

Applications of Group Theory

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Lectures 9.2.01, Mondays, 14:15
Exercises 7.1.21, Fridays, 10:15

Sheet 9

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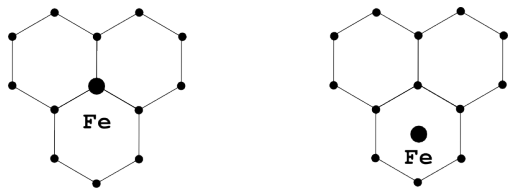
1. Crystal field on an iron impurity

Suppose that an iron (Fe) impurity is introduced into a two-dimensional honeycomb lattice of an insulating host material. A honeycomb lattice is a hexagonal lattice with atoms at the hexagon corners but not at the center of the hexagon.

1. What is the difference in crystal potential (include only nearest neighbors) between the substitutional and he interstitial locations?
2. For the interstitial case, express the results of point 1) in terms of spherical harmonics for the lowest order ter of the potential with angular dependencies.
3. What is the proper point group symmetry and character table in each case?
4. Give the crystal field splitting of the fivefold d-levels of the Fe impurityvin the crystal fields for the two locations introduced in 1).
5. Identify the basis functions associated with each of the levels considered in 4).
6. Since the bonding orbitals lie lower in energy than the antibonding ones, 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!