Lecture Course within the IMPRS „Complex Surfaces in Materials Science“

Group Theory - An Introductory Course with Applications to Molecular and Solid State Physics

Thursday 10^{00} – 11^{30} Fachbereichssitzungssaal, Fachbereich Physik der FU Berlin, Arnimallee 14, 14195 Berlin

Start: Thursday, April 14, 2005

Contents of Lecture Course

1. Symmetry elements and point groups

1.1. Symmetry elements and operations
1.2. Group concepts
1.3. Classification of point groups, incuding the Platonic Solids
1.4. Finding the point group that a molecule belongs to

2. Group representations

2.1. An intuitive approach
2.2. The great orthogonality theorem (GOT)
2.3. Theorems about irreducible representations
2.4. Basis functions
2.5. Relation between representation theory and quantum mechanics
2.6. Character tables and how to use them
2.7. Examples: symmetry of physical properties, tensor symmetries

3. Molecular Orbitals and Group Theory

3.1. Elementary representations of the full rotation group
3.2. Basics of MO theory
3.3. Projection and Transfer Operators
3.4. Symmetry of LCAO orbitals
3.5. Direct product groups, matrix elements, selection rules
3.6. Correlation diagrams

4. Vibrations in molecules

4.1. Number and symmetry of normal modes in molecules
4.2. Vibronic wave functions
4.3. IR and Raman selection rules

5. Electron bands in solids

5.1. Symmetry properties of solids
5.2. Wave functions of energy bands
5.3. The group of the wave vector
5.4. Band degeneracy, compatibility

6. The full rotation group

6.1. Atomic wave functions
6.2. The spherical harmonics
6.3. Selection rules for electron states
6.4. Crystal field splitting