



UNIVERSITÀ  
DEGLI STUDI DI MILANO-BICOCCA

## SYLLABUS DEL CORSO

### Advanced Theoretical Chemistry

2223-94R-SCGA14

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#### Titolo

Advanced Theoretical Chemistry

#### Docente(i)

Piercarlo Fantucci

#### Lingua

English

#### Breve descrizione

1. The discovery of the spin of electrons and other particles. The experiment of Stern-Gerlach. Fine structure of atomic spectra. Schrodinger equation for one and two electrons systems.
2. The exchange symmetry and the exclusion principle. Elementary spin functions for two- and three electrons. General antisymmetric functions in form of determinants.

3. The quantum mechanical description of the spin. Dirac's equations, their reductions and simplifications. Spin properties, Pauli matrices, spin operators and angular momentum operators.
4. The spin and orbital angular momenta. Coupling and the quantum number J. Multiplicity of J components: examples from atomic spectra.
5. Electron spin and wave equations for molecules. Spin-restricted and spin-unrestricted approaches. Eigenfunction of  $S_z$  and  $S^2$ . Spin mixing, spin-projection and spin-annihilation.
6. Electron density and spin density. Local properties of spin density. Long range spin-coupling: ferromagnetism, antiferromagnetism. The solution of the problem of the broken-symmetry. Removal of space-spin degeneracies: the Jahn-Teller theorem.
7. The electron spin and the associated magnetic field. Electron spin in external magnetic field. Zeeman effect.
8. Resonance spectroscopies of electron spin and nuclear spin. Spin-spin coupling.
9. Information on molecular and electronic structures from spin resonance spectra. Examples from organic and inorganic chemistry.
10. Reviews of methods of quantum mechanical calculation of NMR and EPR observables.

Evaluation: YES

### **CFU / Ore**

2,5 CFU - 20 Hours (Lecture)

### **Periodo di erogazione**

II semester

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