UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Advanced Theoretical Chemistry

2223-94R-SCGA14

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, spi 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 Jan-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. Revies 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