An Introduction To Molecular Orbital Theory

6 Lecture Course

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Objectives – a fundamental understanding

- **Wave mechanics / Atomic orbitals**
  - The flaws in classical quantum mechanics (the Bohr Model) in the treatment of electrons
  - Wave mechanics and the Schrödinger equation
  - Representations of atomic orbitals including wave functions
  - Electron densities and radial distribution functions
  - Understanding shielding and penetration in terms of the energies of atomic orbitals

- **Bonding**
  - Revision of VSEPR and Hybridisation
  - Linear combination of molecular orbitals (LCAO), bonding / antibonding
  - Labelling of molecular orbitals (σ, π and g, u)
  - Homonuclear diatomic MO diagrams
  - MO diagrams for Inorganic Complexes

Lecture schedule

Lecture 1	Revision of Bohr model of atoms and an introduction to wave mechanics
Lecture 2	Schrödinger equation, atomic wavefunctions and radial distribution functions of s orbitals
Lecture 3	More complex wavefunctions and radial distribution functions and electron shielding
Lecture 4	Lewis bonding, Hybridisation, and molecular orbitals
Lecture 5	Labelling MO's. 1st row homonuclear diatomics
Lecture 6	MO approach to more complex molecules and CO bonding in transition metals complexes

Information

- Book Sources: all titles listed here are available in the Hamilton Library
  - Chemical Bonding, M. J. Winter (Oxford Chemistry primer 15) Oxford Science Publications ISBN 0 198556942 – condensed text, excellent diagrams
  - Basic Inorganic Chemistry (Wiley) F.A.Cotton, G. Wilkinson, P. L. Gaus – comprehensive text, very detailed on aufbau principle
  - Inorganic Chemistry (Prentice Hall) C. Housecroft, A. G. Sharpe – comprehensive text with very accessible language. CD contains interactive energy diagrams
  - **Additional sources:**

    http://www.shef.ac.uk/chemistry/orbitron/ - plotting AO's