UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Molecular Electronics and Photonics

1819-1-F5302Q017

Aims

The course deals with the physical principles of the properties of molecular semiconductors. Molecular crystals and quantum mechanic origins of the intermolecular forces. Carbon-based policonjugated systems: anisotropy, low-dimensional properties. Polymeric semiconductors.

Contents

ELECTRONIC STATES OF POLICONJUGATED MOLECULES AND POLYMERS.

EXCITED STATES IN MOLECULAR CRYSTALS.

ELECTROLUMINESCENCE AND LED DEVICES.

ORGANIC PHOTOVOLTAIC CELLS.

MOLECULAR ELECTRONICS AND PHOTONICS.

Detailed program

ELECTRONIC STATES OF POLICONJUGATED MOLECULES AND POLYMERS: Free-electron model, Hueckel's model. Band structure of conjugated polymers. Monoelectronic approximation: Su-Shrieffer-Heeger hamiltonian. Electron-phonon interaction and Peierls' gap. Solitons, polarons, bipolarons. Electronic correlation: Hubbard's Hamiltonian. LINEAR OPTICAL PROPERTIES: Absorption and emission of conjugated molecules. Einstein's coefficients and Strickler-Berg's formula. Singlets and triplets. Optical spectra calculation with the "tight-binding" method. Electric susceptibility of ? electrons. Calculation of transition matrix elements. Kasha's rule. Nonradiative processes. Lifetimes. Photoluminescence quantum efficiency and its measurement. EXCITED STATES IN MOLECULAR CRYSTALS: Excited states in molecular aggregates: excitons classification (Frenkel, charge-transfer, Wannier). Delocalization and binding-energy: comparison between organic and inorganic materials. Calculation of the exciton energy. Davydov splitting. Exciton generation mechanisms. Exciton mobility. Coherent and incoherent energy transfer. Foerster's and Dexter's energy transfer. Photonics antenna. ELECTROLUMINESCENCE AND LED DEVICES: Architecture of a prototype device and energetic levels diagram. Injection and charge transport. Exciton generation and recombination. Microcavities. Organic semiconductor-based lasers. ORGANIC PHOTOVOLTAIC CELLS: Organic dye-based photo-electrochemical cells (Graetzel): light harvesting, charge separation and transport. Photoelectrochemical cell efficiency. Organic and polymeric semiconductor cells and their architecture. Charge separation: donors and acceptors. Planar and "bulk" heterojunction. Efficiency. Solar light harvesting optimization: "upconversion" and "downconversion" processes. MOLECULAR ELECTRONICS AND PHOTONICS: use of molecular size structures such as switches, transducers, logic elements, memories. Macro-molecules, biomolecules and supermolecules and their meaning in physics, chemistry and biology. Employment of molecules for photoreactions in biology.

Prerequisites

This course requires a good knowledge of quantum physics (time-independent and time-dependent Schroedinger Equations, perturbation theory, Fermi golden rule), structure of matter (atoms, molecules and solids) and some basic knowledge of organic chemistry.

Teaching form

Lectures

Textbook and teaching resource

T. A. Skotheim, "Handbook of Conducting Pollymers)

J. M. André et. al.," Quantum chemistry aided design of organic polymers"

M. Pope C. E. Swenberg, "Electronic processes in organic crystals"

Several review articles supplied by the lecturer

Semester

2nd SEMESTER

Assessment method

Oral test aimed to verify the capability of the students i) to model and discuss the properties of organic molecules and materials; ii) to analyse the optical end electrical processes occurring in this class of materials; iii) to describe the operation, peculiarities and limits of the electronic and photonic organic devices.

Office hours

By appointment