UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Molecular Electronics and Photonics

2627-1-FSM02Q013

Aims

The course topic is the underhanging of the physics of organic molecular semiconductors, such as conjugated molecules, polymers and advanced hybrid materials, employed in photonics and electronics. In the first part of the course, we will investigate the quantum mechanical description of the electronic properties of these materials from single molecule level to aggregates and solids as well the main mechanisms ruling energy and charge transport in these system. In the second part we will focus on more applicative aspects with an overview on OLED technology, photovoltaics, lasing, super resolution fluorescence imaging techniques and scintillation for detection of ionizing radiation, biomedical applications.

In details, the course has the following Aims:

1. Knowledge and understanding (DnD 1).
   The course aims at teching the physical principles at the base of the electronic, optical and luminescence properties of molecular semiconductors.

2. Applying knowledge and understanding (DnD 2).
   The knowledge acquired at point 1 will be applied to single molecules, molecular crystals, disordered solid system, conjugated polymers adn hybrid systems, and their role in the technology of devices based on conjugated materials.

3. Making judgements (DnD 3).

4. Communication skills (DnD 4).
   Each lesson includes an open discussion with the lecturer to verify and deepen the acquired knowledge, the critical ability to identify the most crucial information, and the capacity to present and communicate it.

5. Learning skills (DnD 5).
   The scientific papers complementing the lectures will also be discussed as examples of research in the literature, to further explore and deepen the topics covered.

Contents

Main topics discussed in the lectures :

1. ELECTRONIC STATES OF POLICONJUGATED MOLECULES AND POLYMERS.
2. EXCITED STATES IN MOLECULAR CRYSTALS.
3. ELECTROLUMINESCENCE AND LED DEVICES.
4. ORGANIC PHOTOVOLTAIC CELLS AND LASERS.
5. FLUORESCENCE IMAGING TECHNIQUES.
6. CONJUGATED SCINTILLATORS FOR THE DETECTION OF IONIZING RADIATION.
7. STATE-OF-THE-ART CONJUGATED AND HYBRID APPLICATIONS IN 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. Calculation of transition matrix elements. Kasha's rule. Non radiative 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. Marcus Theory for charge transport. Photonic antennae.

ELECTROLUMINESCENCE AND LED DEVICES: Architecture of a prototype device and energetic levels diagram. Injection and charge transport. Exciton generation and recombination. Microcavities.

MOLECULAR ELECTRONICS AND PHOTONICS: Physics and architecture of organic light emitting diodes (OLEDs). Light harvesting, charge separation and transport. Organic and polymeric semiconductor cells and their architecture, charge separation: donors and acceptors. Planar and “bulk” heterojunction. Efficiency. Dye-sensitized solar cells based photo-electrochemical cells (Graetzel). Solar light harvesting optimization: “upconversion” and “downconversion” processes. Organic semiconductor-based lasers. Principles and use of organic molecules in fluorescence imaging techniques and super-resolution imaging. Macro-molecules, biomolecules and supermolecules and their meaning in physics, chemistry and biology. Employment of molecules for photoreactions in biology. Physics and use of scitnillation processes in conjugated materials.

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 held in the classroom (30 lectures) through both delivery and interactive methods.
The lecturer will provide in advance the slides that will be the focus of each lesson, along with any scientific articles deemed necessary as complementary material.
In case of requests for further insights, additional material will be prepared and discussed by the lecturer.

Textbook and teaching resource

1. J. M. André et. al.," Quantum chemistry aided design of organic polymers"
2. M. Pope C. E. Swenberg, "Electronic processes in organic crystals"
3. Several scientific papers supplied by the lecturer complementary to the lectures.

Semester

2nd SEMESTER.

Assessment method

Oral test is aimed to verify the capability of the students:
i) to model and discuss the properties of organic molecules and materials;
ii) to analyze 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.

The test will consist in a series of questions regarding:
a) strictly the course program. to assess the acquired knowledge on the general concept and type of materials presented (DnD 1, 2, 5).
b) question more focused on personal interpretation and possible solution of the organic-based device discussed during the lectures. (DnD 3, 4).

The grading scale will be as follows:

Office hours

By appointment, please send an email directly at the lecturere address (angelo.monguzzi@unimib.it).

Sustainable Development Goals

INDUSTRY, INNOVATION AND INFRASTRUCTURE