

## Syllabus

### Course description

<b>Course title</b>	Plastic and Molecular Optoelectronics
<b>Course code</b>	46087
<b>Scientific sector</b>	FIS/01
<b>Degree</b>	PhD in Advanced Systems Engineering
<b>Semester</b>	2
<b>Year</b>	1
<b>Academic year</b>	2024/2025
<b>Credits</b>	3
<b>Modular</b>	No
<b>Total lecturing hours</b>	36
<b>Attendance</b>	Strongly recommended
<b>Prerequisites</b>	Classical mechanics and thermodynamics (Physics I), Electromagnetism (Physics II). Calculus I and II.
<b>Course page</b>	
<b>Specific educational objectives</b>	The student should understand the basic principles of organic, carbon-based semiconductors and apply them to the understanding and design of organic semiconductor devices, with emphasis on optoelectronic ones, such as organic light-emitting diodes (OLEDs) and light-emitting electrochemical cells (LECs), as well as organic photovoltaic diodes (PVDs).
<b>Lecturer</b>	Professor Franco Cacialli Office: Building B1, Room 03.16, NOI e-mail: franco.cacialli@unibz.it tel. 0471 017119 <a href="https://www.unibz.it/en/faculties/engineering/academic-staff/person/47601-franco-cacialli">https://www.unibz.it/en/faculties/engineering/academic-staff/person/47601-franco-cacialli</a>
<b>Scientific sector of the lecturer</b>	FIS/01
<b>Teaching language</b>	English
<b>Office hours</b>	Previous appointment via email
<b>List of topics covered</b>	<b>1) Introduction -</b> <ol style="list-style-type: none"> <li>a. Inorganic semiconductors</li> <li>b. Organic semiconducting (macro)molecules               <ol style="list-style-type: none"> <li>i. <math>\pi</math>-orbitals and conjugation</li> <li>ii. Excitations: excitons and polarons</li> <li>iii. Exciton spin: singlets and triplets</li> <li>iv. Synopsis electronic and optical processes</li> </ol> </li> </ol>

- v. Optical properties: a few examples
  1.  $E_G$  (Energy Gap) vs. molecular weight
  2. Electron-phonon coupling: vibrational structure and thermochromism
  3. Förster transfer and Site-Selective Photoluminescence Spectroscopy
- vi. Summary of optical properties

## 2) Organic light-emitting diodes

- a. Structure
- b. Fundamental processes
  - i. Charge injection
  - ii. Charge transport
  - iii. Exciton formation
    1. Mutual capture
    2. Exciton characteristics (binding energy, spin-multiplicity, capture cross-section)
  - iv. Exciton decay
    1. Radiative and non-radiative decay
    2. Exciton lifetime
    3. Efficiency
- c. Characterisation of OLEDs
  - i. Relevant performance parameters
  - ii. Characterising metal-semiconductor contacts: electroabsorption measurements as a non-invasive tool for the study of the energy level line-up in finished devices
- d. Practical implementations
  - i. Anodes
  - ii. Cathodes
  - iii. Active materials
    1. Singlet emitters
    2. Triplet emitters – enhanced spin-orbit coupling via doping with heavy metals/rare-earth ligands

- 3. Blends: achieving the best of all worlds
  - iv. Fabrication technology: solution processability
- e. State-of-the-art devices and future prospects
  - 1. Thermally activated delayed fluorescence (TADF)
  - 2. Aggregation-induced emission (AIE)
  - 3. Flexible electronics and "tattoo-electronics"

### 3) Organic photovoltaic diodes (PVDs) -

- a. Fundamental process
  - i. Exciton absorption
  - ii. Exciton dissociation
  - iii. Charge collection
- b. Characterisation of PVDs
  - i. Relevant performance parameters
- c. Examples of polymer-based PVDs
  - i. Type II heterojunctions
  - ii. Multi-layers vs. bulk heterojunctions
  - iii. Fullerene and non-fullerene acceptors
- d. State-of-the-art devices and future prospects

### 4) Supramolecular structures -

- a. Introduction to secondary (non covalent) interactions and their role in organic solids
- b. Insulated molecular wires, IMWs and threaded molecular wires (TMWs).
- c. Other types (dendrons).

### 5) Near-infrared (NIR) emitting + absorbing materials

- a. Overview
  - i. Motivation
  - ii. Inorganic or hybrid emitters / absorbers
  - iii. Phosphorescent emitters
- b. Challenges: the energy gap "rule"
- c. Materials not leveraging triplet-assisted photophysics

	d. Current state-of-the-art
<b>Teaching format</b>	The lessons are divided into theoretical classroom lessons and exercises on the blackboard.

<b>Learning outcomes</b>	<p>1. <u>Knowledge and understanding</u>  Knowledge and understanding of:</p> <ul style="list-style-type: none"> <li>- the fundamental physical and chemical properties of organic semiconductors (OS)</li> <li>- <u>Understanding basic operation of organic light-emitting diodes (OLEDs)</u></li> <li>- <u>Understanding basic operation of light-emitting electrochemical cells (LECs)</u></li> <li>- <u>Understanding basic operation of organic solar cells</u></li> </ul> <p>2. <u>Applying knowledge and understanding</u></p> <p>3. Ability to apply knowledge for solving given problems, including solving them with numerical data, approximating significant numbers, and taking care of the notation of units.</p> <p><u>Making judgements</u></p> <p>4. Ability to judge plausibility of results.</p> <p><u>Communication skills</u></p> <p>5. Maturing of technical-scientific terminology.</p> <p><u>Ability to learn</u></p> <p>6. Learning skills to independently study and apply methods of physics for specific applications beyond topics covered in this lecture.</p>
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<b>Assessment</b>	<b>Formative assessment</b>		
	<b>Form</b>	<b>Length /duration</b>	<b>ILOs assessed</b>
	In-class exercises	Continuously as part of course-accompanying exercises	1-6
	<b>Summative assessment</b>		
	<b>Form</b>	<b>Length /duration</b>	<b>ILOs assessed</b>
	Written	120 minutes	1-6
<b>Assessment language</b>	English		
<b>Evaluation criteria and criteria for awarding marks</b>	The exam includes a written (2 hours) and an oral component. The written exam (2 hours) will include 4 questions of either qualitative/semi-quantitative nature as well as		

	<p>numerical or symbolic problems on topics covered in the lectures.</p> <p>The grading will be based on:</p> <ul style="list-style-type: none"> <li>- The correctness of the approach and the mathematical steps of the solution, the calculation of numerical results and the correct use of physical quantities and units.</li> <li>- The correctness of the provided answers and of the presented, as well as the terminology used.</li> </ul> <p>To pass the exam the final grade must be greater or equal to 18. If the final score is greater than 30, a "cum laude" grade is awarded.</p> <p>The student can have access to the exam with pen, pencil and a portable calculator. A short list of constants is provided to the students along with the text of the exam.</p> <p>Depending on the outcome of the written exam students may be invited, at the discretion of the examiner(s), to an oral exam that may include questions on the program covered in the lectures (including those of the written part of the exam) and may lead to an <u>increase or a reduction</u> of the grade of the written component.</p> <p>Students should also be able provide proof of identity (e.g. Campus card, ID card, passport) before the start of the exam.</p>
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<b>Required readings</b>	Course handouts
<b>Supplementary readings</b>	<p>[1] Electronic Processes in Organic Crystals and Polymers, M Pope, C Swenberg, Oxford University Press, 2nd ed., Oxford, 1999</p> <p>[2] <i>Organic Light-Emitting Devices</i>, K Müllen and U Scherf eds., Wiley-VCH, Weinheim, 2006</p> <p><i>Organic Electronics: Foundations to Applications</i>, SR Forrest, Oxford University Press, Oxford, 2020</p>