

CORSI ORGANIZZATI PER L'ANNO ACCADEMICO 2020-2021

Photophysics of Conjugated Organic Materials

Dr. Johannes Gierschner, Madrid Institute for Advanced Studies, IMDEA Nanoscience, Spain

Chromophores, based on conjugated organic molecules, are of eminent importance in chemistry, materials science, biology & pharmacy as functional dyes, pigments and materials in optoelectronics. Analysis of the working principles and design of novel compounds requires however a deep understanding of structure-property relationships in solution and - more challenging - in the solid state, ideally at a predictive level.

In a combined spectroscopic and computational approach, the course (10h) gives a thorough introduction to this subject with a focus on the solid state, however discussing all those molecular concepts which are necessary to understand the modulation of photophysics by intermolecular interactions.

Part 1 "Chromophores in Solution" discusses light-matter interaction, electronic excitations, chemical constitution & absorption, molecular spectra, and excited state deactivation. Part 2 "Chromophores in the Solid State" then discusses concepts of interacting chromophores, homo-/hetero-dimers, weakly coupling 3D assemblies, formation and photophysics of molecular solids, and various organic solid state systems.

[July 2021]

Functional Materials from Photosynthetic Microorganisms

Gianluca M. Farinola, Dipartimento di Chimica, Università degli Studi di Bari Aldo Moro

In the search of sustainable approaches for the production of new materials, the possibility to use photosynthetic microorganisms as a source of functional micro/nano structures opens intriguing possibilities. In fact, combining specialized photosynthetic structures, optimized by billions of years of evolution for specific functions, with tailored molecules paves the way not only to sustainable production methods, but also to intriguing concepts of new materials for photonics, (opto)electronics and bio-medicine.

The course will cover the subject by discussing the following examples:

i) Photosynthetic bacterial enzymes as active materials for photoconversion: their functionalization with molecular antennas and methods for addressing them on electrodes together with applications in photoconverters and phototransistors.

ii) Nanostructures obtained by functionalization of the biosilica shells of diatoms unicellular algae with organic and organometallic molecules and their applications in photonics and in bio-medicine (drug delivery and supports for cells growth).

iii) Living photosynthetic microorganisms as materials for optoelectronics by interfacing them with electrodes.

The course will discuss the concepts of design, synthesis and applications of new materials starting from photosynthetic microorganisms, at the interface of synthetic chemistry, materials science and biotechnology.

[April 2021]

Physical Chemistry of Biomolecules: Applications to Covid-19 proteins

Prof. Paolo Carloni, Institutes for Neurobiology and Medicine (INM-9) and of Advanced Simulation (IAS-5), Juelich Research Center, Juelich, Germany;

Department of Physics, RWTH University of Aachen, Aachen, Germany.

This course (8 h) provides basic concepts on the structure, function, and thermodynamics of proteins, and it illustrates how to get insights on those by simple models as well as by molecular simulation. A basic knowledge of quantum mechanics, statistical mechanics and electrostatics may be useful to appreciate several of the topics presented here. Particularly important are the exercises at the end of the course. These focus on Covid-19 proteins.

The program is divided in four blocks, of 90 minutes each, plus a final session with exercises for the students (2 h).

1. Structural aspects of biomolecules.
2. Thermodynamics basis of proteins' and nucleic acids' structures.
3. Basics elements of molecular simulation and applications to receptor function and enzymatic catalysis.
4. Computer-aided drug design: Application to main targets of SARS-CoV-2. Connection between molecular simulation and systems biology.
5. Exercise for the PhD students: Structural analysis of SARS-CoV-2 Main Protease in complex with inhibitors.

Information on the lecturer's research: http://www.fz-juelich.de/ias/ias-5/EN/Home/home_node.html

[Jan-Feb 2021]

Synthetic approaches to the development of new Antibody-Drug Conjugates

Prof. Elena Petricci, Dipartimento di Biotecnologie, Chimica e Farmacia, Università degli Studi di Siena

The course aims to furnish the basic knowledge of the major issues on the design and development of new Antibody Drug Conjugates (ADC) for different purposes.

The course is organized into four units (approximately 2 h each) covering the following topics:

- (1) basic introduction to bioconjugation and ADC;
- (2) issues in ADC design: linker, payload and anchoring approaches;
- (3) ADC technology in cancer therapy. Case studies: use of HDAC or Smo inhibitors as payloads;
- (4) ADC technology beyond cancer.

[Spring 2021]

Diffraction methods in materials science

Prof. Marco Taddei

The discovery that crystals can diffract X-rays, made by Max von Laue in 1912, sparked a revolution in the study of solid-state materials, giving scientists a precious tool to “see” the atomic structure of matter. This course aims at providing an exhaustive overview of diffraction-based methods for the characterization of solid-state materials and will cover the following topics:

- I) Basic concepts of crystallography: crystals, unit cell, symmetry operations, Bravais lattices, Miller indices, reciprocal lattice. Diffraction of X-rays by crystalline solids.
- II) Generation and detection of X-rays. Single crystal X-ray diffraction: structural analysis. Powder X-ray diffraction: indexing, whole powder pattern fitting, structure solution, Rietveld method.
- III) Powder X-ray diffraction: quantitative phase analysis, microstructural analysis, thin films analysis, textural analysis. In situ X-ray diffraction.
- IV) Diffraction by nanocrystalline/amorphous materials: total scattering techniques. Neutron diffraction. Electron diffraction.

[September 2021]