SIMN Modules

Academic Year: 2022-2023

Modules Overview

The date(s) of the Courses are continuously update. To enroll, go to the Moodle page of the PhD Course at the link:

https://stem.elearning.unipd.it/course/index.php?categoryid=501

#	Module Title	Instructor(s)	Dept.	hrs	Session 1 (Jan-Mar 2023)	Session 2 (June-July 2023)	Session 3 (Sept. 2023)	Course Program
1	Broadband Electric Spectroscopy	Di Noto	DII	8				*The basic principles and applications of Broadband Electric Spectroscopy will be presented.*
2	Chemisorption and physisorption in the characterization of powder catalysts	Glisenti	DiSC	8		July 3-4, 2023		*Chemisorption and physisorption based methods are precious for the1) characterization of solid phase catalysts. Temperature Programmed Reduction and Oxidation allow to describe the type, amount and distribution of active sites for the activation of molecules; 2) safe and sustainable storage and transportation of hydrogen 3) carbon dioxide activation.*
3	Contact angle and surface tension measurements	Ferraro	DFA	8		July 2023		*Contact angle and surface tension measurements are technique used to evaluate the interfacial properties of liquids and solid surfaces (wetting), which are very common in both research and industrial activities. In the first case, they are typically employed to characterized new type of "smart" coatings, while in the second to verify the homogeneity chemical-physical properties of the surface.* *In this course, the various strategies for characterizing the contact angle of a surface and the surface tension of a liquid will be presented, showing several examples from both academic and industrial fields. Different examples of smart coating will also be presented taken from the literature in order to highlight the main chemical-physical parameters that control these interfacial phenomena. Example of measurements will be presented with a setup installed at the Department of Physics and Astronomy.*
4	DLS & Z potential	Carraro	DiSC	8				*The basic principles of Dynamic Light Scattering and Z-Potential techniques will be presented.*

								Examples will be covered and group work will allow to solve and discuss case studies.
5	Dynamic Mechanical Analysis and Modulated Differential Scanning Calorimetry	Di Noto	DII	8				*The basic principles and applications of Dynamic Mechanical Analysis and Modulated Differential Scanning Calorimetry will be presented*
6	Electrochemical Methods for the ex-situ Characterization of Energy Storage Materials	Di Noto – Pagot	DII	8				*The proposed course will cover briefly the most important aspects of electrochemistry with a major emphasis on its application in materials for the reversible energy storage. The objective is to provide an understanding of the fundamentals of the electrode reactions and of the principles of electrochemical methods.* *The use of voltamperometric techniques will be discussed to describe the insertion/de-insertion and the deposition/stripping processes occurring during the redox reactions of active materials in an electrochemical cell. The attention will be devoted on how the reversibility, efficiency, overpotential and kinetics of such reactions can be gauged by means different ex-situ electrochemical methods. Moreover, a description of the principal ac techniques, such as the electrochemical impedance spectroscopy (EIS), will be given, with a particular reference on how they can provide information on the changes in the cell properties during cycling. In details, EIS can supply in-depth details on the evolution of the electrode-electrolyte interfaces. Finally, the course will focus its attention on the device testing of different active materials under specific procedures, thus achieving a deeper understanding on the peculiarities of the investigated compounds. In this fragment, several examples of electrochemical devices for the reversible storage of energy will be taken under consideration.* *In summary, the lectures and the discussion will give an insight in applications of several electrochemical methodologies. These will be followed by laboratory exercises which will give a hands-on experience of real electrochemical experiments.*
7	Ellipsometry	Martucci	DII	8				*The course will give the basic priciples of elliposmetry.* *Examples of different types of thin films will be presented*

8	High-Resolution X-Ray Diffraction and X-ray Reflectivity	Bazzan - De Salvador	DFA	8				*The basic principles of HR-XRD and XRR will be discussed. Some data taking and analysis example will be given.*
9	Mass Spectrometry and Nuclear Magnetic Resonance for the identification of organic compounds	Sartorel	DiSC	8		July 27-28, 2023		*The basic principles and applications of Mass Spectrometry and Nuclear Magnetic Resonance will be presented. Case studies will be discussed, for the identification of organic compounds and materials.*
10	Materials Modeling with Quantum Espresso	Silvestrelli	DFA	8		June 16, 2023		*This course presents some basic features of the Quantum ESPRESSO ab-initio computational package. Quantum ESPRESSO (http://www.quantum-espresso.org/) is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials, and runs on almost every conceivable current computer architecture. In the first part of the course a general description of the computational package is given, together with basic installation information, and illustrations of different applications (both at basic level and concerning recent research activities): electronic band structures and phonon dispersion curves of crystals and 2D materials, optimization of molecular structures, visualization of electron-charge density profiles,... The second part is instead devoted to practical activity: the students will install the Quantum ESPRESSO package on their own computers and try to reproduce some of the applications presented in the first part. The acquisition of the basic competencies will be certified by a final exam (evaluation questionnaire).*
11	Methods and instrumentation for the study of surface area and density of solids	Vezzù	DII	8				*This course presents the principles of density and surface area measurements by gas techniques such as pycometer and BET (Brunauer, Emmett and Teller).* *In the first part of the course a general description of techniques will be present.* *The second part is instead devoted to practical activity: in small groups, the participants will be able to see how BET and the gas pycnometer work.*

								Moreover, each group would perform a density measurement on a solid sample of interest.
12	Microfabrication techniques	Ferraro	DFA	8	March 2023			*Microfabrication refers to the set of processes needed for realizing structures having micrometer size. Historically, it was developed during the second half of the 20th century from the electronics industries, pushing the production of smaller and smaller devices. Nowadays, due to the develop of the micro-mechanics and optics, new strategies of microfabrication are risen a lot of attraction, e.g.: 3D printing.* *In this course, the most important microfabrication strategies will be presented, including photo- and soft- lithography, 3D printing, micro-injection molding, presenting several examples taken from the literature. Some real examples of the introduced techniques will also be presented, exploiting the facilities presented at the Department of Physics and Astronomy.*
13	Optical Tweezers	Merano - Zaltron	DFA	8				*The basic principles of optical tweezers will be presented.*
14	Photothermal heating	Amendola	DiSC	8	Jan. 25, 2023			*Photothermal heating is involved in a wide range of scientific phenomena and technological applications. For instance, laser-matter interaction is studied for biomedical applications or for triggering structural and chemical processes in heat-responsive systems. Of great relevance in the contemporary efforts for a sustainable future, sunlight-driven photothermal heating is exploited for distillation, desalination, evaporation up to thermal photovoltaics.* *This course consists of two parts: first, an overview of photothermal applications, related materials, and the basics of the photothermal heating physics will be provided; then, students will be divided in groups and will participate in a laboratory part for the measurement of photothermal heating curves in an absorbing nanofluid and data analysis.* *Verification: Report with the fitting of heating curves and calculation of the light-to-heat conversion efficiency (group report) + 1 page resume of a scientific article about photothermal heating appeared in the last 2 years (single student report).*

15	Powder and Thin-Film X-ray Diffraction	Gasparotto	DiSC	1				*The course aims at providing PhD Students a general overview about X-ray diffraction techniques for the structural analysis of materials, with special emphasis to powder and thin film systems. Besides introducing X-ray diffraction from a theoretical point of view, the course will also focus on practical issues, e.g. describing the main components of commercial diffractometers, considering sample preparation issues, and practicing on data elaboration and interpretation.*
16	SEM: Scanning Electron Microscopy	Maccato	DiSC	1				*The basic principles of Scanning Electron Microscopy will be presented*
17	STM: Scanning Tunneling Microscopy	Sedona - Carlotto	DiSC	8		June 26-30, 2023		*The principles and applications of the scanning tunneling microscopy (STM) will be presented and then applied in a case study: iron phthalocyanines deposited on metal surfaces before and after the oxygen dosage. The course can be divided in two parts: i) a practical part in which the surfaces will be prepared and characterised on a UHV system and ii) a part in which DFT modelling will be used to interpret the experimental results.* *Prof. Sedona* *- Scanning Tunneling Microscopy (STM) and Tunneling Spectroscopy (TS:) a brief overview of the operating principles. (1h)* *- Experimental practice: deposition of iron phthalocyanines on a metal substrate under UHV conditions and STM characterization. (3h max 4 students)* *Prof. Carlotto* *- Connection between periodic calculations and STM measurements (1h)* *- Description of a periodic calculations input file for QuantumEspresso (1h)* *- Analysis of the optimised structures for metal (iron) phthalocyanines on metal surfaces before and after oxygen dosage: geometrical parameters, DOS and PDOS and charge density (1h)* *- STM simulations at different bias of the different optimised structures (1h)*
18	UV-VIS-NIR Optical Spectroscopy and Raman scattering	Meneghetti	DiSC	8	Feb. 17, 2023			*The principles and the instrumentation of the exctinction in the UV-Vis-NIR spectral regions and those of the Raman scattering are reviewed and applied in laboratory*
19	XPS: X-ray Photoelectron Spectroscopy	Agnoli - Cattelan - Rizzi	DiSC	8		July 2023		*electron spectroscopies: XPS and Auger electron spectroscopy* *the photoemission process: matrix element, cross sections, the sudden approximation model*

								the binding energy: elemental and chemical shift, auger parameter *shape of photoemission peaks: electronic effects (spin orbit), final state effects, anelastic losses* *quantitative analysis by xps: sensitivity factors* *instrumentation of xps: UHV environment, electron analyzer, x-ray source* *examples of analysis of photoemission spectra (calculation of inelastic mean free path, peak fitting, background substraction)*