PhD in Physical and Chemical Sciences (40th cycle): list of courses and related syllabi

1) Advanced microscopy and spectroscopy techniques applied to nanomaterials - (I year - II sem.)

The course (20 hours duration) will be held in the period March-July 2025
(Ref. 1) S. Agnello – simonpietro.agnello@unipa.it; 2) G. Buscarino – gianpiero.buscarino@unipa.it)

Description: *Introduction to advanced Atomic Force Microscopy (AFM) and Raman spectroscopy, and their use in material science.*

Contents

• *Fundamentals and applications of the Atomic Force Microscopy.*

• *Tip-surface interaction forces.*

• *Introduction to the main AFM scanning modes.*

• *Theory of Amplitude Modulation Atomic Force Microscopy.*

• *Overview of the AFM instrumental setup.*

• *Overview of vibrational spectroscopy: normal modes of molecules and solids.*

• *Raman spectroscopy: Elastic and inelastic scattering.*

• *Molecular vibration and polarizability. Classical and semiclassical approach to Raman effect.*

• *Instrumental setups and microscopy tools.*

Notes: *The training activity provides laboratory experiments: i) determination of the size distribution of nanoparticles distributed on a flat surface; ii) application of the Micro-Raman technique.*

2) Time resolved spectroscopy and microscopy - (I year - II sem.)

The course (20 hours duration) will be held in the period March-July 2025.
(Ref. 1) M. Cannas – marco.cannas@unipa.it; 2) A. Sciortino – alice.sciortino@unipa.it)

Description: *Time-resolved photoluminescence spectroscopy and microscopy, and their use in material science.*

Contents

• *Overview of luminescence phenomena: intrinsic and extrinsic properties of solids; size dependence effects in nanomaterials.*

• *Basic design of experimental setups for nanosecond-picosecond resolved experiments: pulsed laser sources; time-resolved detectors*

• *Time-resolved photoluminescence experiments: design and interpretation of the data.*

• *Time-resolved micro-luminescence experiments: design and interpretation of the data.*

Notes: *The training activity provides laboratory experiments: i) acquisition of time resolved photoluminescence spectra of model systems; ii) time-resolved micro-luminescence of model systems.*

3) Organic/Inorganic Nanocomposites: thermodynamics, structure, and applications - (I year - II sem.)
The course (20 hours duration) will be held in the period March-July 2025
(Ref. G. Cavallaro – giuseppe.cavallaro@unipa.it)

Description: *Presentation of the techniques employed for the thermodynamic and structural characterization of organic/inorganic nanocomposites. Correlation between the mesoscopic properties and the potential applications for Cultural Heritage, packaging, remediation and pharmaceutics.*

Contents
• Preparation of nanocomposite materials in aqueous, gel and solid phases.

• Thermodynamic characterization:

• Differential scanning calorimetry (DSC): basic concepts, experiments and data analysis. First and second order transitions. Crystallinity degree.

• Isothermal titration calorimetry (ITC): basic concepts, experiments and data analysis. Thermodynamics of interactions: entropy, enthalpy, Gibbs free energy and stoichiometry. Van't Hoff equation vs ITC experimental data.

• Dynamic mechanical analysis (DMA): basic concepts, experiments and data analysis. Mechanical and viscoelastic properties.

• Thermogravimetry (TGA): basic concepts, experiments and data analysis. Thermogravimetric and differential thermogravimetric curves.

• Kinetic studies by non-isothermal TGA experiments: isoconversional procedures

• Structural characterization by light and neutron scattering techniques

• Correlation between the structure and the mesoscopic properties. Barrier effect on the thermal resistance. Mechanical behaviour, transparency and water uptake ability. Control of the hydrophobic/hydrophilic character of the surfaces.

• Nanocomposites for cultural heritage conservation: surface cleaning protocols and consolidation/deacidification of lignocellulosic artworks. Nanocomposites for environmental purposes: biocompatible packaging and decontamination. Nanocomposites for pharmaceutical applications: controlled delivery of active molecules.

Notes:*. The course consists of both frontal lectures and laboratory activities.*

4) Introduction to DFT and TDDFT - (I year - I sem.)
The course (20 hours duration)will be held in the period November 2024 – February 2025.
(Ref. U. De Giovannini – umberto.degiovannini@unipa.it)

Description: *Introduction to the basic concepts and theorems of DFT and TDDFT, and hands-on experiences to the use of the Octopus DFT/TDDFT code.*

Contents - Theory
• The Hohenberg-Kohn theorem

• The Kohn-Sham approach

• The Runge-Gross theorem

• Introduction to linear response theory

• Optical properties of electronic systems with TDDFT

Contents -Hands-on tutorials with the Qctopus code

• Finite systems

• The ground state of benzene molecule

• The absorption cross-section of benzene form real-time TDDFT

• Periodic systems

• The band structure of graphite

• The optical conductivity with real-time TDDFT

5) **Open quantum systems dynamics** (I and II year - II sem.)
The course (20 hours duration) will be held in the periods March- July 2025 and March- July 2026.
(Ref. 1) S. Lorenzo – salvatore.lorenzo@unipa.it; 2) L. Innocenti – luca.innocenti@unipa.it)

Description: ***1)*** *Introduction to Open Quantum Systems Dynamics using the programming language Python;*
2) *Theoretical and practical introduction to Quantum machine learning*

Contents - Part 1)
• *Python and Quantum Physics:*
• *States and Operators*
• *Density operator, Partial Traces and Superoperators*
• *Quantum Dynamical Maps*
• *Positive and Complete Positive Maps, Operator-sum representation*
• *Markovian Semigroup*
• *Open Quantum System Dynamics*
• *Master Equation*
• *Stochastic Master Equation (Monte Carlo Method)*
• *Collision models*

Contents - Part2)
• *Basic notions of machine learning:*
• *Different learning paradigms (unsupervised, supervised, reinforced), different models (types of neural networks)*
• *Different training methods (stochastic gradient descent and its variants)*
• *Basic notions of quantum computation relevant to understand efficiency claims.*
• *Quantum-enhanced machine learning vs machine learning applied to quantum: the many different ways to merge machine learning and quantum information science.*
• *Some case studies of problems arising in quantum information theory which can be tackled with machine learning.*

6) **Experimental techniques in astroparticle physics -** (I year - II sem.)
The course (20 hours duration) will be held in the period March- July 2025.
(Ref. 1) G. Marsella – giovanni.marsella@unipa.it; 2) M. Mallamaci manuela.mallamaci@unipa.it)

Description : *Principal experimental techniques in astroparticle physics*.

Contents
• *Introduction to Cosmic Ray (CR) sources*
• *Primary CRs, acceleration mechanism, propagation*
• *Secondary CRs, atmospheric showers*
• *Detection techniques in Space, Extensive Air Shower arrays and underground detectors*
• *Presentation of the principal experiments and recent results*

7) Numerical methods for out-of-equilibrium statistical physics - (I year - II sem.)
The course (20 hours duration) will be held in the period March-July 2025.
(Ref.1 D. Valenti – davide.valenti@unipa.it2) P. Lazzari – gplazzari@ogs.it)

Description*: Numerical methods to study out-of-equilibrium systems and noise induced effects in physical and inter-disciplinary contexts.*

Contents
• *Wiener process and stochastic differential equations.*

• *Use of FORTRAN** language to devise numerical methods for studying and modeling nonlinear physical systems.*

• *Numerical methods for solving stochastic differential equations in the presence of nonlinear potentials (Gaussian noise). Noise induced effects: stochastic resonance, noise enhanced stability.*

• *Numerical implementation of algorithms for the pseudo-random generation of Lévy noise.*

• *Applications to physical and interdisciplinary systems.*

• *Deterministic and stochastic models applied to population dynamics with complex interactions, an example from a marine ecosystem mode*

• *Stability, periodicity, chaos and interaction with noise in a complex ecosystem model, numerical applications with Python*

Notes:*. The will be done in collaboration with Istituto Nazionale di Oceanografia e Geofisica Sperimentale (OGS),Trieste. - In alternative to FORTRAN, students attending the course can use C or Python. Lectures on the final part of the program will begiven on line. The learning assessment will be through a talk/discussion, which deepens a topic related to the course and/or to the research interests of the student.*

8) Extrasolar Planets - (I year - II sem.)
The course (20 hours duration) will be held in the period March- July 2025.
(Ref. G. Micela – giusi.micela@inaf.it)

Description: *Properties and analysis methods of exoplanets*

Contents
• *Exoplanet context*

• *Definitions and background*

• *Stars, brown dwarfs, and planets*

• *Exoplanet detection*

• *Radial velocity method*

• *Transiting planets*

• *Population properties*

• *Atmospheres*

• *Analysis techniques*

• *Instrumentation available today*

• *Future ground and space instrumentation*

9) Project Management in the Scientific-Spatial Context - (II year - I sem.)
The course (20 hours duration) will be held in the period November 2025 - February 2026.
(Ref. G. Micela – giusi.micela@inaf.it)

Description: *Introduction to best practices in managing complex scientific projects, in particular space projects*

Contents

- *Projects and Programs*
- *Basic concepts of management*
- *Space Projects*
- *The main actors of space science*
- *The phases of a project*
- *Feasibility analysis*
- *Requirements & budgets*
- *Model Philosophy*
- *Methods and planning tools for complex projects*
- *The role of the project manager*
- *The relevance of documentation*
- *The correct communication*
- *Financial reporting*

10) Astrophysics laboratory of thermal X-ray plasmas (I year - II sem.)
The course (20 hours duration) will be held in the period March- July 2025.
(Ref. C. Pinto – ciro.pinto@inaf.it)

Description: *Introduction to the properties of thermal X-ray plasmas, techniques of line diagnostics, and application to X-ray spectra from astrophysical sources.*

Contents

- *Elements of atomic physics, binding energy and chemical abundances*
- *Ionization balance in collisional and photo-ionized plasmas*
- *Thermal continuum and spectral lines emission*
- *X-ray detectors with moderate to high spectral resolution*
- *Collisional processes in stellar coronae and hot plasmas*
- *Photo-electric processes in warm winds from binary stars*
- *Absorption processes in the hybrid, multi-phase, interstellar medium*
- *Monte Carlo methods, line detection, and spectra simulations*

Notes: *The activity is developed through 4 hours of frontal lectures and 16 hours of laboratory in which the students consolidate their knowledge through practical exercises of X-ray spectra modelling.*

11) Millisecond Pulsars: Theory and Observations - (I and II year - I sem.)

The course (20 hours duration) will be held in the periods November 2024 - February 2025 and November 2025 - February 2026.
(Ref. R. Iaria – rosario.iaria@unipa.it)

Description: *Introduction to the properties of Millisecond Pulsars, isolated and in binary, and their evolutive connections.*

Contents
- *Classification and basic properties of isolated and binary millisecond pulsars, and emission mechanisms*
- *Formation and evolution: the recycling scenario*
- *Theory of spin and orbital evolution*
- *Spectral and timing properties of Accreting Millisecond pulsars*
- *Evidences of non conservative mass transfer*

12) Introduction to agent-based models - (I year - I sem.)

The course (20 hours duration) will be held in the period. November 2024 - February 2025.
(Ref. S. Miccichè – salvatore.micciche@unipa.it)

Description: *The course will provide basic concepts about agent-based models with an emphasis on their origin and their applications. The contributions from statistical physics to the understanding and solution of ABMs will also be discussed by considering toy-models such as the Ising model on a lattice. Applications in physics, social sciences and economy will also be considered.*

Contents
Part 1: Introduction to Agent-Based models
- *Agent-based model in sociology*
- *Agent-based models in finance and economics*
- *Agent- Based models in transportation systems*

Part 2: Statistical Physics and Agent-Based models
- *Statistical Physics of minority game*
- *Mean-field theories and agent-based models*
- *The Ising model and its social interpretation.*

Part 3: Applications
- *Netlogo*
- *Calibration and validation*
- *Review of popular ABMs*
- *Schelling model, epidemic spreading, predator-prey systems*
- *Voter model, sznajd model, kim-markowitz model*

Notes: *The course is organized in 10 lectures of approximately 2 hours each. In general, the lectures will provide basic concepts on a specific topic. Students will be then requested to carry on some coding activities aiming at numerically solving simple problems related to the topics dealt with during the lectures.*

13) Long Range correlations in statistical physics (I year - II sem.)

The course (20 hours duration) will be held in the period March- July 2025.

(Ref. S. Miccichè – salvatore.micciche@unipa.it)

Description: *The course will provide basic concepts concerning long-range interactions in stochastic processes and Hamiltonian systems, in order to emphasize the importance of these interactions in statistical mechanics.*

Contents

Part 1: Long-range correlations in continuous stochastic processes

- *Introduction to stochastic processes. Langevin equation as a motion equation in presence of noise*
- *Langevin equation and Fokker-Planck equation*
- *Eigenfunctions methodology*
- *Memory properties in stochastic processes. Doob theorem*
- *Ergodicity of log range correlated processes*
- *Extreme value theory*

Part 2: Long-range correlations in discrete stochastic processes

- *Markov chains*
- *Hidden Markov Models*
- *ARCH e GARCH stochastic processes*
- *FbM, ARIMA, FARIMA, FI-GARCH stochastic processes*

Part 3: Long-range interactions in statistical mechanics

- *Mean field theories*
- *Hamiltonian systems with long range interactions*
- *Quantum systems with long-range interactions*
- *Out-of-equilibrium long-range correlations*

Notes: *Students will be requested to carry on some coding activities aiming at numerically solving simple problems related to the topics dealt with during the lectures. The evaluation will be done through the discussion of an assignment related to one of the topics discussed during the module.*

14) Quantum field theory in a curved spacetime or in non-inertial frames (I and II year - I sem.)

The course (20 hours duration) will be held in the periods November 2024 - February 2025 and November 2025 - February 2026.

(Ref. 1) R. Passante roberto.passante@unipa.it; 2) L. Rizzuto lucia.rizzuto@unipa.it)

Description: *Introduction to field quantization in a curved spacetime or in a non inertial frame, or with moving boundaries, and related effects.*

Contents

- *Second quantization of a massless scalar field in a curved spacetime or in a noninertial reference frame*
- *Field quantization with moving boundary conditions.*
- *Extension to the quantum electromagnetic field.*
- *Particle production in a time-dependent gravitational background and cosmological implications*
- *Macroscopic quantum electrodynamics and medium-assisted bosonic field operators.*
- *Dynamical Casimir and Casimir-Polder effect with oscillating dielectric or metallic boundaries.*
- *Quantum friction.*
- *Unruh and Hawking effects.*
- *Quantum thermodynamics of black holes.*

15) Quantum optics & topology in photonic lattices (I year - II sem.)
The course (20 hours duration) will be held in the period March- July 2025.
(Ref. 1) F. Ciccarello – francesco.ciccarello@unipa.it; 2) A. Carollo –angelo.carollo@unipa.it)

Contents
• *Band structure, Topology and Symmetry. Bulk-Edge correspondence*
• *Paradigmatic examples: SSH model (1D), Rice-Mele model (1D), Haldane model (2D)*
• *Topological interpretation of quantum Hall effect*
• *Berry curvature, and Chern number*
• *General approach to topological classification of crystals based on symmetries*
• *Resolvent method and self-energy*
• *Photonic lattices and crystals*
• *Spontaneous emission close to a photonic bandgap*
• *Atom-photon bound states*
• *Adiabatic elimination*
• *Effective many-body Hamiltonians mediated by photons*
• *Vacancy-like atom-photon bound states*

Notes: *The activity is developed through frontal lectures with some exercises.*

16) Quantitative and Qualitative Analysis Methods in Physics Education Research (II year - II sem.)
The course (20 hours duration) will be held in the period March- July 2026.
(Ref. C. Fazio – claudio.fazio@unipa.it)

Contents
• *The research paradigms in behavioral sciences*
• *Construction and validation of a questionnaire.*
• *Reliability and consistency quantitative analysis and contexts of use*
• *Descriptive statistics and inferential statistics*
• *Choice and use of various techniques*
• *Parametric and non-parametric statistical tests*
• *Correlation measures and significance tests*
• *Classical test theory, content analysis, factor analysis, cluster analysis, implicative analysis, similarity analysis, test response theory, model analysis*
• *Qualitative analysis and contexts of use: interview protocols and related analysis*
• *Semantic analysis of the content*
• *Multi-method analysis*
• *Discussion on application examples in physics education research*

17) Quantum Information Theory and Quantum Computing (I year - II sem.)

The course (20 hours duration) will be held in the period March- July 2025.

(Ref. 1) M. Paternostro - mauro.paternostro@unipa.it 2) G. M. Palma – massimo.palma@unipa.it)

Contents

• Density operators, Bloch vectors, bipartite systems and reduced density operators, Schmidt decomposition. Von Neumann entropy.

• Entanglement separability and non-locality ,entanglement quantifiers, quantum discord.

•Quantum Key Distribution, quantum teleportation, superdense coding

• Discrete dynamics of open systems and completely positive maps, Kraus representation, quantum channels, depolarizing channel, dephasing. POVM, channel capacity.

• Quantum computing, quantum logic gates, quantum algorithms: Deutsch, Deutsch-Jozsa, quantum Fourier transform, Grover.

• Elements of measurement-based quantum computation

18) Hetero-geneous Catalysis: Computational and Experimental Perspectives (I year - II sem.)

The course (20 hours duration) will be held in the period March- July 2025.

(Ref. L. Lisuzzo lorenzo.lisuzzo@unipa.it)

Description*: This course will deal with both general aspects and specific case studies about heterogeneous catalysis from the model design in silico to the catalyst synthesis in vitro and chemo-catalytic conversion.*

Contents

• Definition of catalytic process. Homogeneous, heterogeneous, enzymatic catalysis.

• Introduction to the most used methods for the study of catalysis in computational chemistry.

• Catalyst modeling and design: computational screening as an alternative to reduce experimental waste.

• Experimental preparation of catalyst in lab. How to exploit the computational findings for an efficient preparation?

• Catalyst characterization techniques: FTIR, thermogravimetry, optical and electronic microscopies, active sites identification, etc.

• The catalytic process: from reagents to products. Computational study of the reaction mechanism. Experimental conversion and efficiency assessment.

19) XPS: materials and biomaterials analysis and applications (I year - I sem.)
The course (20 hours duration) will be held in the period November 2024 - February 2025
(Ref. M. Scopelliti michelangelo.scopelliti@unipa.it)

Description*: Introduction to X-Ray Photoelectron Spectroscopy (XPS) technique and its application in the fields of material science, including the application to biomaterials.*

Contents
- *Fundamentals of the technique*
- *Ultra-High Vacuum technologies*
- *Instrumental setup*
- *Sample preparation and sample handling*
- *Common analysis routines*
- *Mapping and profiling*
- *Data analysis*

Notes*: Course activities comprehend both frontal lectures and laboratory activities.*

20) Femtosecond science and nonlinear optics - (I year - II sem.)
The course (20 hours duration) will be held in the period March-July 2025.
(Ref. 1) F. Messina – fabrizio.messina@unipa.it; 2) A. Sciortino – alice.sciortino@unipa.it)

Description: *Introduction to nonlinear ultrafast optical spectroscopies and their applications in material science.*

Contents
- *Basics of nonlinear optics*
- *Generation, propagation and control of femtosecond light pulses.*
- *Overview of ultrafast time-resolved spectroscopies in the visible-UV range*
- *Femtosecond Pump/Probe spectroscopy.*
- *Femtosecond Fluorescence upconversion spectroscopy.*

Notes: *The training activity consists in laboratory experiments involving femtosecond time-resolved pump/probe spectroscopic analysis of model systems.*

21) Non Hermitian Hamiltonians and related topics - (I year - I sem.)

The course (20 hours duration) will be held in the period November 2024 – February 2025.

(Ref. F. Bagarello – fabio.bagarello@nipa.it)

Description: *We will discuss several aspects of quantum systems described by non Hermitian Hamiltonians..*

Contents

• *Mathematical preliminaries: Hilbert spaces, Biorthogonal bases, Bounded and unbounded operators*

• *Deformed commutation relations: ladder operators arising from different commutation rules, and from their deformations*

• *Coherent states for pseudo-bosons: bicoherent states and quantization of classical systems*

• *Dynamics for non Hermitian Hamiltonians: transition probabilities; Schroedinger and Heisenberg dynamics; symmetries; constants of motions; algebraic dynamics; derivations.*

• *Distributions and quantum mechanics: weak pseudo-bosons; weak bicoherent states*

• *Physical models: applications to physical models: shifted harmonic oscillator; Supersymmetric pseudo-bosonic potentials; inverted harmonic oscillator*

22) Advanced Materials and Technologies for Photovoltaics - (I year - II sem.)

The course (20 hours duration) will be held in the period March-July 2025.

(Ref. V. Ferrara – vittorio.ferrara@unipa.it)

Description: *The course aims to provide an overview of the fundamental principles of the sciences and technologies for photovoltaics, starting from the basic concepts of the physical chemistry of materials, to the description of next-generation solar cells and the physicochemical processes involved.*

Contents

• *Properties of semiconductor materials, energy band model*

• *Photovoltaic effect, current generation mechanisms, and charge transport*

• *Solar cells: generations of cells, junctions, materials used, operating mechanisms, thin-film technology, structure of photovoltaic panels*

• *Manufacturing and physicochemical characterization techniques of materials and devices*

• *Innovative technologies and cutting-edge materials in photovoltaic research.*

Notes: *The course consists of 10 frontal lessons of 2 hours each, during which the physicochemical properties and processes of the materials used for solar cells will be highlighted in order to understand their functioning and the strategies pursued for further advancements in the field of solar energy.*

23) Introduction to Conformal Field Theories- (I year - II sem.)
The course (20 hours duration) will be held in the period March-July 2025.
(Ref. G. Lo Monaco – gabriele.lomonaco@unipa.it)

Contents
• *Path integrals and renormalization group flow*

• *Scale invariance and the conformal group in D>2*

• *Representations of the conformal group*

• *Constraints of conformal symmetry on correlators*

• *Radial quantization and the state-operator correspondence*

• *The conformal group in D=2 and the Virasoro algebra*

• *The Calabrese-Cardy formula*

• *The SYK model.*

24) Magnetohydrodynamics in Astrophysical Processes - (II year - I sem.)
The course (20 hours duration) will be held in the period November 2025 – February 2026.
(Ref. S. Colombo – salvatore.colonbo@inaf.it)

Description: *This course provides an in-depth understanding of hydrodynamics, magnetohydrodynamics (MHD), and radiative hydrodynamics formulations, with a focus on their application in astrophysical phenomena.*

Contents
Theoretical Part
• *Introduction to Hydrodynamics(HD) and Magnetohydrodynamics(MHD: 1) Fundamentals of HD and MHD formulations; 2). Key equations and principles*

• *Radiative Hydrodynamics: 1) Introduction to radiative transfer equations in hydrodynamics; 2) Importance in astrophysical contexts*

• *Instabilities in Astrophysical Flows: 1) Rayleigh-Taylor Instabilities; 2) Kelvin-Helmholtz Instabilities*

• *Magnetohydrodynamic Shocks: 1. Overview of MHD shocks; 2) Their role and significance inastrophysical processes*

Practical Part
• *High-Performance Computing(HPC) in Astrophysics:1) Introduction to HPC for MHD simulations; 2) Overview of commonly used MHD codes in astrophysics*

• *Detailed Study of the PLUTO Code: 1) In-depth exploration of the PLUTO code; 2) Hands-on development of a PLUTO setup*

• *Exploring Configurations and Solutions in the PLUTO code: 1) Experimentation with different configurations; 2) Analysis of their effects on the solutions*

• *Final Project: 1) Development of a custom MHD setup; 2) Presentation of the setup and results to the committee*

Notes: *The Final Project will be the subject of the final exam.*