



PhD in Physical and Chemical Sciences (38th cycle): list of courses and related syllabi

- 1) **Advanced microscopy and spectroscopy techniques applied to nanomaterials** (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 spectroscopies 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 course (20 hours duration) is active in the first year. The training activity provides laboratory experiments: i) determination of the size distribution of nanoparticles distributed on a flat surface; ii) application of the MicroRaman technique.

- 2) **Advanced time resolved spectroscopy** (Ref. 1) M. Cannas – marco.cannas@unipa.it; 2) F. Messina – fabrizio.messina@unipa.it)

Description: Introduction to fast (ns) and ultrafast (fs) photoluminescence spectroscopies 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 setup: pulsed laser sources; time-resolved detectors
- Overview of ultrafast time-resolved spectroscopy.
- Generation, manipulation and use of ultrashort light pulses.
- Basics of nonlinear optics

Notes: The course (20 hours duration) is active in the first year. The training activity provides laboratory experiments: i) acquisition of time resolved photoluminescence spectra of model systems; ii) pump/probe spectroscopy



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3) Organic/Inorganic Nanocomposites: thermodynamics, structure, and applications (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 pharmaceuticals.

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 (20 hours duration) is active in the first year; it consists of both frontal lectures and laboratory activities.

4) Numerical methods for out-of-equilibrium statistical physics (Ref. D. Valenti – davide.valenti@unipa.it)

Contents

- Dynamics of a Brownian particle subject to an oscillating bistable potential: stochastic resonance
- Use of FORTRAN language (in alternative, students attending the course can use C or Python) 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 enhanced stability. Dynamics of a Brownian particle subject to an oscillating bistable potential: stochastic resonance.
- Numerical methods for advection-reaction-diffusion equation with noise terms: modeling of natural systems.
- Numerical implementation of algorithms for the pseudo-random generation of Lévy noise.
- Numerical methods for solving stochastic differential equations in the presence of nonlinear potentials (Lévy noise).
- Application in physical and real systems (interdisciplinary context)

Notes: The course (20 hours duration) is active in the first year.



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- 5) **Open quantum systems and quantum machine learning** (Ref. 1) S. Lorenzo – salvatore.lorenzo@unipa.it;
2) L. Innocenti – luca.innocenti@unipa.it)

Description: **Part 1** Introduction to Open Quantum Systems Dynamics using the programming language Python;
Part 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

Part 2)

- 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.

Notes: The course (20 hours duration) is active in the first year.

- 6) **Experimental techniques in astroparticle physics** (Ref. G. Marsella – giovanni.marsella@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

Notes: The course (20 hours duration) is active in the first year



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7) Extrasolar Planets (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*

Notes: *The course (20 hours duration) is active in the first year*

8) Project Management in the Scientific-Spatial Context (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*

Notes: *The course (20 hours duration) is active in the second year.*



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9) Introduction to DFT and TDDFT (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

Hands-on tutorials with the Qctopus code

- Finite systems
- The ground state of benzene molecule
- The absorption cross-section of benzene from real-time TDDFT
- Periodic systems
- The band structure of graphite
- The optical conductivity with real-time TDDFT

Notes: The course (20 hours duration) is active in the first year

10) Astrophysics laboratory of thermal X-ray plasmas (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 course (20 hours duration) is active in the first year. 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.



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11) Millisecond Pulsars: Theory and Observations (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

Notes: The course (20 hours duration) is active in the first and in the second year.

12) Introduction to agent-based models (Ref. S. Micciché – 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 (20 hours duration) is active in the first year. It 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.



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13) Quantum field theory in a curved spacetime or in non-inertial frames (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 noninertial 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.

Notes: The course (20 hours duration) is active in the first year.

14) Quantum optics & topology in photonic lattices (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 course (20 hours duration) is active in the first year. The activity is developed through frontal lectures with some exercises.



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15) Quantitative and Qualitative Analysis Methods in Physics Education Research (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*

Notes

The course (20 hours duration) is active in the second year.

16) Quantum Information Theory and Quantum Computing (Ref. G. M. Palma – massimo.palma@unipa.it)

Contents

- *Density operators, Bloch vectors, bipartite systems and reduced density operators, Schmidt decomposition. VonNeumann entropy.*
- *Entanglement separability and non-locality, entanglement quantifiers, entanglement of formation, discord.*
- *Quantum Key Distribution, quantum teleportation, quantum dense 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.*
- *Neuromorphic quantum computation*

Notes

The course (20 hours duration)