PhD in Physical and Chemical Sciences (39th 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*

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 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 (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.1 D. Valenti – davide.valenti@unipa.it) 2) G. Cottone – grazia.cottone@unipa.it

Description: *Numerical methods for stochastic processes as tools to describe out-of equilibrium nonlinear systems and noise induced effects.*

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.*

• *Application in real systems (interdisciplinary context)*

• *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).*

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

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. 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*

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

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.*

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 form 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.*

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. 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 (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.*

13) Long Range correlations in statistical physics (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 and complex systems.*

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: *The course (20 hours duration) is active in the first year. It is organized in 14 lectures of approximately 1.5 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.*
The evaluation of the student 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

(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.*

15) 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.*

16) 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.

17) 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)) is active in the first year.

18) Hetero-geneous Catalysis: Computational and Experimental Perspectives

(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.*

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

19) X-Ray Photoelectron Spectroscopy - materials and biomaterials analysis and applications

(Ref. M. Scopelliti michelangelo.scopelliti@unipa.it)

Description: *Introduction to the 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: *The course (20 hours duration) is active in the first year. Course activities comprehend both frontal lectures and laboratory activities.*