PhD in Physical and Chemical Sciences: 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. 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.*

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*

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*
- *Ionisation balance in collisional and photo-ionised 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) 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.*

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.