UNIVERSITY of CAGLIARI
Department of Physics

RESEARCH PLAN 2013-2015
of the
DEPARTMENT of PHYSICS

as approved on December 17th, 2012

Address: **Dipartimento di Fisica** - Cittadella Universitaria, 09042 Monserrato (Ca)
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UNIVERSITY of CAGLIARI
Department of Physics

INDEX

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UNIVERSITY of CAGLIARI
Department of Physics

1. OUTLOOK

The Department of Physics (DSF) of the University of Cagliari (UniCa) is the only academic institution in Sardegna which mission is addressed to research and higher education in the domain of physical sciences. As such, DSF will play a key role in promoting culture, formation, and research in physics with large impact on the regional system.

At present, the DSF research staff consistens in:

- 8 full professors (PO)
- 14 associate professors (PA)
- 18 tenured assistant professors (RC-TI)
- 3 non-tenured assistant professors (RC-TD)

In addition, the DSF workforce is completed by about ten Post Docs, about twenty Ph.D. students, and about ten graduate students in medical physics.

Based on experimental, theoretical, and computational research activities, DSF will develop new advanced knowledge (curiosity-driven as well as application-oriented) in high-energy, condensed matter, and applied physics, as well as in astrophysics.

Full detail about any research line, the network of national and international collaborations, and the list of ongoing projects is reported in this document.
Research plans are grouped according to the "Domain" and "Sub-domain" system adopted by the Italian Ministry for University and Research (MiUR) and they are listed, with reference to the principal investigator, in alphabetical order. In addition, they are labeled according to the classification scheme adopted by the "European Research Council" (ERC).

DSF will guest and collaborate with the local sections of Italian Institute of Nuclear Phsyics (INFN), the Italian Istitute of Astrophysics (INAF), and two institutes belonging to the National Council of Research (CNR), namely: the Institute "Materials Forgery" (IOM) and the Institute for Atmospheric Sciences and Climatology (ISAC).

2. RESEARCH DOMAINS ACCORDING TO "EUROPEAN RESEARCH COUNCIL" (ERC)
The research activities here presented are labeled according to the general classification scheme of "European Research Council" (ERC).
Below is reported the ERC synopsis for the physical sciences.

PE2 Fundamental constituents of matter:
particle, nuclear, plasma, atomic, molecular, gas, and optical physics

PE2_1 Fundamental interactions and fields
PE2_2 Particle physics
PE2_3 Nuclear physics
PE2_4 Nuclear astrophysics
PE2_5 Gas and plasma physics
PE2_6 Electromagnetism
PE2_7 Atomic, molecular physics
PE2_8 Optics and quantum optics
PE2_9 Lasers and laser physics
PE2_10 Acoustics
PE2_11 Relativity
PE2_12 Classical physics
PE2_13 Thermodynamics
PE2_14 Non-linear physics
PE2_15 General physics
PE2_16 Metrology and measurement
PE2_17 Statistical physics (gases)

PE3 Condensed matter physics:
structure, electronic properties, fluids, nanosciences

PE3_1 Structure of solids and liquids
PE3_2 Mechanical and acoustical properties of condensed matter
PE3_3 Thermal properties of condensed matter
PE3_4 Transport properties of condensed matter
PE3_5 Electronic properties of materials and transport
PE3_6 Lattice dynamics
PE3_7 Semiconductors
PE3_8 Superconductivity
PE3_9 Superfluids
PE3_10 Spintronics
PE3_11 Magnetism
PE3_12 Nanophysics: nanoelectronics, nanophotonics, nanomagnetism
PE3_13 Mesoscopic physics
PE3_14 Molecular electronics
PE3_15 Soft condensed matter (liquid crystals…)
PE3_16 Fluid dynamics (physics)
PE3_17 Statistical physics (condensed matter)
PE3_18 Phase transitions, phase equilibria
PE3_19 Biophysics

PE4 Physical and Analytical Chemical sciences:
analytical chemistry, chemical theory, physical chemistry/chemical physics

PE4_1 Physical chemistry
PE4_2 Nanochemistry
PE4_3 Spectroscopic and spectrometric techniques
PE4_4 Molecular architecture and Structure
PE4_5 Surface science
PE4_6 Analytical chemistry
PE4_7 Chemical physics
PE4_8 Chemical instrumentation
PE4_9 Electrochemistry, electrodialysis, microfluidics
PE4_10 Combinatorial chemistry
PE4_11 Method development in chemistry
PE4_12 Catalysis
PE4_13 Physical chemistry of biological systems
PE4_14 Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions
PE4_15 Theoretical and computational chemistry
PE4_16 Radiation chemistry
PE4_17 Nuclear chemistry
PE4_18 Photochemistry

PE5 Materials and Synthesis:
materials synthesis, structure-properties relations, functional and advanced materials, molecular architecture, organic chemistry

PE5_1 Structural properties of materials
PE5_2 Solid state materials
PE5_3 Surface modification
PE5_4 Thin films
PE5_5 Corrosion
PE5_6 Porous materials
PE5_7 Ionic liquids
PE5_8 New materials: oxides, alloys, composite, organic-inorganic hybrid, superconductors
PE5_9 Materials for sensors
PE5_10 Nanomaterials : nanoparticles, nanotubes
PE5_11 Biomaterials synthesis
PE5_12 Intelligent materials – self assembled materials
PE5_13 Environment chemistry
PE5_14 Coordination chemistry
PE5_15 Colloid chemistry
PE5_16 Biological chemistry
PE5_17 Chemistry of condensed matter
PE5_18 Homogeneous and heterogeneous catalysis
PE5_19 Characterization methods of materials
PE5_20 Macromolecular chemistry,
PE5_21 Polymer chemistry
PE5_22 Supramolecular chemistry
PE5_23 Organic chemistry
PE5_24 Molecular chemistry

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UNIVERSITY of CAGLIARI
Department of Physics

RESEARCH PLAN

Domain "High-energy physics"

Sub-domain 02A1 "Experimental high-energy physics"

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Production and characterization of the quark gluon plasma in ultra-relativistic heavy ion collisions

2. Principal investigators
Alessandro De Falco, Gianluca Usai

3. Research team

Full professors	Giovanna Puddu
Associated professors	Gianluca Usai
Assistant professors	Alessandro De Falco
Post docs	Cristina Terrevoli
Ph. D. students	Ester Casula, Alberto Collu, Elisa Incani, Masha Razazi, Sabyasachi Siddhanta
INFN researchers	Alberto Masoni (Direttore di Ricerca), Corrado Cicalò (Primo Ricercatore)

4. ERC (European Reserach Council) research classification scheme

PE2_1	PE2_2	PE2_3

5. Key words

Heavy Ion Collisions	Quark Gluon Plasma	ALICE LHC

6. National and international collaborations on this topic
The team is part of the ALICE international collaboration, LHC, CERN. It collaborates with CERN groups, French groups (Saclay, Nantes, Strasburgo, Lione), Torino (INFN, University), Padova (INFN, University), Bari (INFN, University), Heidelberg.

7. Abstract
The team research is focused on the experimental program of the ALICE experiment at the CERN LHC. For the 2013-2105 period, the activities will range from the study of muon pairs to the design of a new silicon pixel detector. The team will also study a new spectrometer to measure muon production at low energies at the CERN SPS.

8. Framework and state-of-the-art
In a ultra-relativistic heavy ion collision (Pb-Pb or Au-Au), a large number of nucleons interact depositing a large energy (of the order of 1 GeV) in a rather small volume (of the order of 1 fm^3). This can lead to the production of a plasma with deconfined quarks and gluons, having properties similar to the plasma formed in the first stages of the Universe birth, around 3ms after the big bang. In the last 20 years, the properties of the quark gluon plasma were studied first at the CERN SPS and then at the RHIC collider at BNL. Presently the LHC can accelerate heavy ions at the largest energy ever reached (2.76 TeV/nucleon). Several experiments (ALICE, CMS e ATLAS) are performing new important measurements in this new unexplored energy regime.

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9. Research description, milestones, and goals

The research team is partecipating to heavy ion experiments, in particular focused on muon pair production, since 15 years. Muon pairs can be produced from the decays of light mesons as the r(770), ω(780) e f(1020) or heavier as the J/ψ(3100), whose properties can be substantially modified by the plasma medium. The production of charm and beauty is also very interesting since it allows one to study the production, propagation and hadronization mechanisms of heavy quarks in the dense nuclear medium produced in the heavy ion collisions.

ALICE experiment - The ALICE experiment is a world-wide involving more than 80 research institutes and about 1000 researchers.

During 2013 a new measurement of proton-Pb collisions will be performed. Within the approved experimental program, the research team will be involved in the following activities:

- Data taking proton-Pb
- Development of computing infrastructures based on the GRID technology for data analysis and data reconstruction.
- Study of low mass dimuon production in Pb-Pb collisions ($m<1.2$ GeV/c^2)
- Development of techniques for the combinatorial background subtraction in the dimuon mass spectrum.
- Maintainance of the Muon Arm and Zero Degree Calorimeters (ZDC) detectors.

Besides those activities, the team is also involved in the proposal for the construction of a new pixel vertex detector. The project was approved by the LHCC scientific committee during the 2012 fall. This detector will allow one to measure with high precision the production of charm and beauty mesons and baryons. The team will be involved in the following activities:

- Study of the production of beauty baryons
- Study and characterization of new pixel detectors

Responsibiities within the collaboration:

- Conveener of the working group in charge for defining the new experimental program in the period 2018-2025 with the new pixel detector and editor of the Letter of Intent (G. Usai)
- Conveener of the Physics Analysis Working group in charge for the analysis of low mass muon pairs (A. De Falco)

A. De Falco is responsible for the Cagliari unit of the project PRIN *Development of computing technologies for the optimisation of access to LHC data and for the technology transfer towards other research areas using the grid and cloud computing approach*.

NA60 experiment - The NA60 experiment at the CERN SPS has been directed by G. Usai and will finish the experimental program focused on the proton-nucleus data in 2013. G. Usai is responsible for a PRIN project *Chiral symmetry restoration and search of the QCD critical point: measurements of dilepton production in nuclear collisions at the CERN SPS* has been approved devoted to study a new spectrometer to extend the measurements performed by NA60 to the enery interval 20-160 GeV/nucleon. The team will be involved in the following activities:

- Monte Carlo simulations of the experimental apparatus to optmize the pixel and muon tracking stations
- Study of low mass dimuon production as a function of energy in the interval 20-160 GeV/nucleon Sand as a function of centrality.

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Physics of quarks and leptons: Heavy Flavours at LHCb and Polarized targets for neutrino experiments.

2. Principal investigator
Biagio Saitta

3. Research team

Professors	Biagio Saitta
Associated professors	
Assistant professors	Giulia Manca, Rudolf Oldeman
Post docs	
Ph. D. students	

4. ERC (European Research Council) research classification scheme

PE2_1	PE2_2	

5. Key words

Flavour physics	LHC	Neutrinos

6. National and international collaborations
- W. Bonivento, S. Cadeddu, A. Cardini, A. Contu, and A. Lai, researchers from the local section of the Istituto Nazionale di Fisica Nucleare (INFN) operating under the framework agreement between INFN and the University of Cagliari, are integral part of the group.
- For the LHCb experiment: INFN, CERN and about 50 Institutions from 14 different countries (Europe, Brazil, China, US)
- For the neutrino project: University and INFN Padova.

7. Abstract
During the next three years the group will pursue a wide range of topics related to the physics of heavy flavours, using data collected by the LHCb experiment at CERN, addressing in particular production cross-sections, charm physics and rare decays of both charmed and B-mesons. In addition the group will contribute to the foreseen upgrade of the experiment, taking advantage of the expertise of some of its members in the development of detectors and electronics. It is also expected that the studies on the feasibility of polarized targets for neutrino physics will reach completion on a similar time scale, setting the basis for a larger scale experiment.

8. Framework and state-of-the-art
Flavour physics is at the heart of several long-standing fundamental questions of particle physics and cosmology: What is the origin of the asymmetry between matter and antimatter in the universe? What is the solution of the hierarchy problem, the mechanism that quantum corrections to the mass of the Higgs boson require extreme fine tuning to separate it from the Planck scale? The yield of particles containing b-quarks at the LHC is now an order of magnitude higher than achieved so far at any previous accelerator and therefore it is possible to perform a wide range of measurements of unprecedented precision and to search for very rare decay modes.

In the Standard Model of electroweak interactions, left-handed neutrinos interact mainly with left-handed electrons (or nuclei), owing to the V-A Lorentz structure of the current. A new generation of neutrino experiments could stem from the exploitation of this feature - so far unused – which makes it possible, by controlling the polarization of the target, to alter the rate of weak interactions.

9. Research description, milestones, and goals

LHCb – analyses. In 2012, LHCb recorded 2.0 fb-1 of pp collisions, twice as much as in 2011, and at a slightly higher energy of 4.0TeV per beam (3.5TeV in 2011). This new, larger data sample will be used both to update and improve existing measurements and to start new analyses. In particular it is foreseen:

- To update and extend the already published Upsilon production cross-section with the inclusion of measurements of its polarization and of the excited states χ_b (including the recently discovered χ_b(3P) state, whose production cross-section has never been measured).
- To analyse the decay of the neutral D-meson into two muons and two pions, taking advantage of the excellent muon identification capabilities of the LCHb detector with the intent of setting the best world limit on this decay mode, similar to that obtained in 2012 for $D \rightarrow \mu\mu$.
- To complete the development of novel methods to identify the presence of the charmed baryon Λc in a decay without the need to reconstruct it, thus enabling a measurement of its absolute decay branching fractions, very poorly known so far.
- To set limits on the lepton flavour violating decay mode $B_s \rightarrow \mu\tau$.

LHCb –upgrade. A major upgrade of the LHCb experiment is being prepared for the data taking periods from 2019 onwards, in which it is envisaged that the detector will be read out at 40MHz instead of the present 1 MHz. This will allow running at 2.5 to 5 times the present luminosity, increasing the efficiencies for hadronic B decays. The group is involved in the upgrade of the muon detection system which requires a modification of the electronics used for the readout. Furthermore, if tests that are underway demonstrate that the inner regions of the upstream muon detectors loose efficiency at high luminosity, it might prove necessary to develop new, high-granularity detectors (like triple Gas Electron Multipliers) as well as new digital front-end electronics.

Several members of the group have recognised leadership roles within the international collaboration and therefore are in a position to ensure the achievement of these goals.

Neutrinos. R & D studies towards the realisation of a neutrino target/detector, in which the polarization state of the electrons is controlled by an external magnetic field, have demonstrated in 2012 that it is possible to obtain about 80% of the maximum allowed polarization by placing small GSO scintillating crystals in a magnetic field of 4T at cryogenic temperatures of about 4K. It is planned:

- to extend the measurements to larger crystals already available;
- to detect (using a SQUID), synchronously with the scintillation, the signal due to the change in magnetisation caused by the energy deposited in the GSO crystals by electrons or photons;
- to complete the studies on the performance at low temperatures of avalanche photodiodes (APD);
- to simulate the effects of new types of neutrino interactions (right-handed currents, magnetic moment) to estimate in a quantitative manner the advantage of having a polarised target.

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UNIVERSITY of CAGLIARI
Department of Physics

RESEARCH PLAN

Domain "High-energy physics"

Sub-domain 02A2 "Theoretical high-energy physics"

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Black holes and the gravity/gauge theory correspondence

2. Principal investigator
MARIANO CADONI

3. Research team

Full professors	
Associated professors	MARIANO CADONI
Assistant professors	
Post docs	
Ph. D. students	MATTEO SERRA

4. ERC (European Reserach Council) research classification scheme

PE2_1	PE2_11	

5. Key words

Black holes	gravity/gauge theory correspondence	

6. National and international collaborations on this topic
P. Pani, IST , Lisbon, Portugal; S. Mignemi, Dip. Mathematics University of Cagliari

7. Abstract
We plan to use the gravity /gauge theory correspondence to investigate several interesting hot problems of high energy theoretical physics:

1. Holographic description of critical systems
2. Domain wall/cosmology correspondence
3. Non perturbative features of QCD
4. Microscopic entropy of black holes and other extended objects

8. Framework and state-of-the-art
In the large N limit the conjectured string theory in AdS/gauge theory correspondence reduces to a duality between Anti-de Sitter (AdS) gravity in the bulk and a quantum field theory (QFT) in the boundary (gravity/ gauge theory correspondence). In this form the duality is power tool from two different points of view. On the one side, it allows to describe holographically strongly coupled QFTs just by investigating a classical theory of gravity. On the other side, it allows to gain information on the semiclassical regime of interesting gravitational systems such as black holes by investigating dual QFTs. In fact in recent years this correspondence has been used to tackle, holographically, a wide variety of problems ranging from superconductors, charge transport features of metals, critical systems, nonperturbative features of QCD, derivation of microscopic and entanglement entropy of black holes. The power of holographic methods is far reaching and represents a promising tool for solving several hot problems of high energy theoretical physics.

UNIVERSITY of CAGLIARI
Department of Physics

9. Research description, milestones, and goals
The research activity in the next three years will be focused on different aspects, problems and applications of the gravity /gauge theory correspondence. Here is a short description of the different research lines.

1. Holographic description of critical systems

(In collaboration with M. Serra, P. Pani)
Recently it has been shown that hyperscaling violation is a quite generic holographic feature of broad classes of Einstein-Maxwell-scalar gravity with fields coupled in several ways when the potential behaves exponentially. Our aim is to give a general holographic description of the Hyperscaling violation in critical system. This will be achieved working both on the gravity bulk side (for instance by working out analytical or numerical solutions) and the QFT side (for instance by computing critical exponents and transport features) of the duality.

2. Domain wall/cosmology correspondence

(In collaboration with S. Mignemi)
One interesting feature of a broad class of Einstein-scalar gravity, which have been investigated by us in recent times, is the existence of solitonic domain wall (DW) solutions interpolating smoothly between an AdS spacetime and of scale-covariant metric. On the other hand the conjectured domain wall /cosmology correspondence implies that these solutions should have a time-dependent counterpart that could be very interesting for cosmological applications (for instance inflation and the dark energy problem). Our main goal here is to derive the cosmological solutions dual the DW and to investigate their features.

3. Non perturbative features of QCD

(In collaboration with G. D'Appollonio and U. D'Alesio and F. Murgia (INFN))
The aim of this research line is to use the gravity/gauge theory duality for understanding nonperturbative features of QCD, in particular hadronic structure functions and other spin observables in hadronic processes at high energy. In particular we plan to analyze hadron scattering in holographic models for understanding spin asymmetries along to two main lines: a) investigation of hadronic correlators in the dual theory; b) Investigation of azimuthal asymmetries and of single spin with particular attention to the non perturbative mechanisms that could originate them.

4. Microscopic entropy of black holes and other extended objects

Within this research line we plan to use the gravity/gauge theory correspondence for computing both the statistical entropy and the entanglement entropy of black holes. Although in recent years we have seen improvement in this direction, there are still many unsolved open problems. In particular, we aim to gain a better understanding of the relationship between the three black hole entropies: thermodynamical, statistical (Boltzmann), entanglement (Von Neumann).

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UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
3-dimensional structure of the nucleon and transverse-single spin asymmetries

2. Principal investigator
Umberto D'Aleso

3. Research team

Assistant professor	Umberto D'Alesio

4. ERC (European Research Council) research classification scheme

PE2_1	PE2_2	

5. Key words

Nucleon structure	Partonic intrinisic motion	Quark and gluons (QCD)

6. National and international collaborations on this topic
F. Murgia (INFN-Ca), M. Anselmino, M. Boglione (Torino), A. Prokudin (Jefferson Lab, USA), E. Leader (Imperial College, UK), I. Scimemi (Univ. Complutense, Madrid, Spain), experimental groups (PAX, COMPASS, HERMES, JLAB, STAR, PHENIX, BELLE, BABAR).

7. Abstract
- Extraction of transverse momentum distributions (TMDs) from experimental data in SIDIS and e^+e^- processes, with their proper Q^2 evolution;
- Role of TMDs in single spin asymmetries (SSAs) for single-inclusive hadron and jet-hadron production in proton-proton collisions;
- TMDs and SSAs within the gauge-string duality

8. Framework and state-of-the-art
The interpretation of the lepton-nucleon high-energy scattering data within the QCD parton model has contributed fundamentally to our present knowledge about the nucleon structure. This information is encoded in the so-called Parton Distribution Functions (PDFs) - extracted from data and non-calculable - which give the number density of partons inside a proton with a longitudinal momentum fraction x. However, many other important and interesting aspects of the structure of the nucleon are not revealed by the standard PDFs. They do not address questions such as: Do quarks orbit? How are they spatially distributed inside the proton? Is there a connection between the motion of quarks, their spin and the spin of the proton?
A serious and systematic attempt to answer the above questions started about a decade ago, with both dedicated experiments and new theoretical ideas. The crucial innovation is that of looking at, and studying, physical observables which are sensitive to the transverse structure of the nucleon. For fast moving protons, the transverse properties (with respect to their direction of motion), both in spin and motion, give novel information. This, when combined with the available longitudinal information, allows a truly 3-dimensional understanding of the proton structure, encoded in the TMDs. Moreover, these functions result fundamental for a description of single spin asymmetries which cannot be understood within the usual collinear factorization theorems at leading twist.
This research activity will address mainly these two related issues.

9. Research description, milestones, and goals

The TMDs contain information on the intrinsic motion of quarks and gluons inside a fast moving nucleon. When adding the spin degree of freedom, they also link the parton spin to the parent proton spin and to the parton intrinsic momentum. Among the 8 independent TMD at leading twist, besides the 3 surviving in collinear limit, the most studied ones are the Sivers and the Boer-Mulders functions, which give, respectively, the density number of unpolarized (transversely polarized) partons inside a transversely polarized (unpolarized) proton. Similar correlations can occur in the fragmentation process; for instance, the Collins function gives the number density of unpolarized hadrons resulting from the hadronization of a transversely polarized quark.
In all analysis of TMDs performed so far the QCD evolution has been taken into account at a simplified level. Thanks to latest achievements this evolution can be now included in a systematic and correct way into the data analysis of semi-inclusive deep inelastic scattering (SIDIS) and e^+e^- annihilation processes. A global fitting procedure will be developed by implementing dedicated numerical codes. [12-18 months]

Several Single-Spin Asymmetries (SSAs) have been observed, since a long time and at different energies, in inclusive hadronic interactions, such as $pp \rightarrow \pi X$, where one of the protons is transversely polarized and the pion is produced with a large transverse momentum (p_T). A phenomenological description of these asymmetries, based on the generalization of the collinear factorization approach to the case of TMDs, has been developed with a good phenomenological success. The issue of whether or not the same Sivers and Collins functions, as extracted from data in processes for which factorization has been proved to hold (like SIDIS), might contribute to the SSAs in pp is still open and will be under investigation. [9-12 monts]
The study of single-jet production at large p_T in pp collisions will continue: here, by looking at the azimuthal distribution of pions inside the jet, one can separately consider the role of the Sivers and Collins effects and study their universality. [4-6 months]
We will also complete a phenomenological analysis of the latest RICH data at central rapidities leading to a new constraint on the gluon Sivers function.
[4-6 months]

In collaboration with M. Cadoni, G. D'Appollonio (U. Cagliari) and F. Murgia (INFN-Ca) a complementary research activity on the gauge-string duality will be started. The aim will be a better understanding of nonperturbative features of QCD, like parton distribution function, TMDs and other spin observables in hadronic processes at high energy. In particular, we plan to analyze hadron scattering in holographic models for understanding spin asymmetries along to two main lines: a) investigation of hadronic correlators in the dual theory; b) Investigation of azimuthal and single spin asymmetries with special attention to the nonperturbative mechanisms that could originate them. [12-18 months]

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UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
String dynamics in curved spacetimes and at high energy

2. Principal investigator
Giuseppe D'Appollonio

3. Research team

Full professors	
Associated professors	
Assistant professors	
Post docs	
Ph. D. students	

4. ERC (European Reserach Council) research classification scheme

PE2_1	PE2_2	

5. Key words

Strings and D-branes	AdS/CFT	Higher spin fields

6. National and international collaborations on this topic
Paolo Di Vecchia, Nordita, Stockholm, Sweden;
Rodolfo Russo, Queen Mary, University of London, London, UK;
Gabriele Veneziano, Collège de France, Paris, France.

7. Abstract
This research project is devoted to the study of string theory in two closely related contexts: in the proximity of its characteristic scale, the Planck scale, and in curved spacetimes possessing a microscopic description, such as those sourced by a collection of D-branes. Through the analysis of the string scattering amplitudes, we will clarify the quantization of the string in an external metric and the gauge symmetries and interactions of the higher spin field theories.

8. Framework and state-of-the-art
The symmetries of string theory represent a vast generalization of the gauge and diffeomorphism invariances which are familiar from quantum field theory. These symmetries and their dynamical consequences are not manifest in perturbation theory. In a similar way it is not evident in perturbation theory how string theory circumvents the difficulties that arise in the semiclassical approach to quantum gravity, the main one being how to reconcile a unitary evolution with the semiclassical properties of the black hole metric. The string S matrix in the high energy limit is a natural starting point to address these problems, as emphasized in the past by D. Amati, M. Ciafaloni and G. Veneziano and by D. Gross and F. Mende.

9. Research description, milestones, and goals

In its perturbative formulation string theory defines, order by order in the coupling constant, the S matrix of a relativistic quantum theory of an infinite number of fields of increasing mass and spin. The structure of the theory is highly constrained, reflecting the consistency conditions which must be fulfilled in order to introduce a fundamental length scale in a relativistic theory. The only possible string interaction is indeed the joining and splitting of strings in a three-string vertex, a process already included in the Polyakov integral which defines the S matrix. The uniqueness of the theory at the microscopic level is in sharp contrast to the huge variety of possible vacuum states, namely the classical solutions of the equation of motion that describe the configuration of the massless fields. The perturbative evaluation of the spectrum and of the scattering amplitudes requires the choice of a ground state and, in particular, of a metric.

A natural setting to study the symmetries of string theory and the space-time singularities is the high energy limit. In this limit the string tension becomes negligible and all the vibration modes effectively massless. We will evaluate elastic and inelastic string scattering amplitudes, both at fixed angle and at fixed momentum transfer. They will represent our main tool to identify the degrees of freedom relevant at high energy, to clarify the structure of the interaction vertices of the higher spin field theories and to study the conjectured symmetry breaking mechanism that should lead to the appearance of the Planck scale, leaving the gauge symmetry unbroken only in the massless sector.

The high energy limit coincides with the strong coupling limit of the gravitational interactions and allows the study of the classical and quantum string corrections to general relativity. We will approach this problem by analysing two simple but paradigmatic processes: the collision of two strings at Planckian energies and the scattering of a string in the background sourced by a collection of D-branes. From a semiclassical point of view both processes imply a loss of unitarity, due in the first case to the formation of a black hole and in the second to the disappearance of the string in the singularity. A complete treatment of these processes in string theory should enable us to establish the existence of a unitary S matrix and to understand the details of the microscopic dynamics which is described only in an approximate way by the quantization in the external metric.

The study of the dynamics of string theory in curved spacetimes finds many important applications also in the context of the string/gauge duality. According to this correspondence, the string spectrum and scattering amplitudes in a spacetime dual to a gauge theory capture the behavior of the field theory in the region of strong coupling. In collaboration with M. Cadoni, U. D'Alesio and F. Murgia (INFN-CA) we will study some non-perturbative aspects of field theory models which are similar to QCD and possess a dual string description. We will focus on possible effects at the origin of the spin asymmetries and on the form of the parton distribution functions at small x.

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Exotic neutrino interactions and new short baseline oscillations experiments

2. Principal investigator
Alberto Devoto

3. Research team

Full professors	
Associated professors	Alberto Devoto
Assistant professors	
Post docs	
Ph. D. students	

4. ERC (European Reserach Council) research classification scheme

PE2_3	PE2_2	

5. Key words

neutrino	sterile	Non standard

6. National and international collaborations on this topic
Laboratori Nazionali del Gran Sasso, Princeton University

7. Abstract
Calculation of the consequences of the existence of sterile neutrinos on future short baseline oscillations experiments

8. Framework and state-of-the-art
Neutrino cross sections within the realm of the standard model are well established and are available in the literature. The available data offer a base for the analysis of neutrino oscillations data which will be available in the near future.

Address: **Dipartimento di Fisica** - Cittadella Universitaria, 09042 Monserrato (Ca)
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9. Research description, milestones, and goals

We intend to take into account the consequence of the existence of one or more sterile (non standard model) neutrinos and the signature that they would leave on future short-baseline neutrino oscillation experiments.

UNIVERSITY of CAGLIARI
Department of Physics

RESEARCH PLAN

Domain "Condensed matter physics"

Sub-domain 02B1 "Experimental condensed matter physics"

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UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
NeOS, Neuronal Optical Spectroscopy: measuring the brain activity with light

2. Principal investigator
Alberto Anedda

3. Research team

Full Professors	Alberto Anedda, Gian Luigi Gessa
Assistant professors	Marcello Salis
Post docs	Marco Marceddu

4. ERC (European Reserach Council) research classification scheme

PE4_3	PE3_19	LS5

5. Key words

optical spectroscopy	biophysics	neuroscience

6. National and international collaborations on this topic
Dr Giancarlo Colombo, CNR Neuroscience Institute, Cagliari

7. Abstract
This research project claims to investigate the possibility to develop a new optical spectroscopy technique for the measurement of the brain and neuronal activity, with particular attention to the identification and localization of tissue areas devoted to "like" and "dislike" mental states.

8. Framework and state-of-the-art
Functional Near Infra Red Spectroscopy (fNIR) is regarded as a very promising approach to the development of non a invasive technique able to provide a functional imaging of the brain activity. This technique employs a light beam to probe specific areas of the brain, while reacting to external stimuli, thus providing the identification and localisation of tissue areas devoted to specific cognitive tasks. Measurement are performed by analysing the optical charateristics (amplitude, phase modulation) of the diffused NIR light beam interacting with the brain area, where an event-related is expected to increase of the neuronal activity.
A different but more intriguing, strategy may focus on the detection of the diffused radiation of pulsed excitation (50-200 ms) that might be associated to changes of the optical properties during neuronal firing, due to mutations in the membrane potential or in the cellular volume.
The actual experimental technique can monitor the change in oxyhaemoglobin (O_2Hb) and deoxyhaemoglobin (HHb) that accompany neuronal activity.
The physiological foundation of this approach relies on the interaction between neuronal activity and haemodinamics and oxygenation.

9. Research description, milestones, and goals

This research project claims to point out the brain functions and neuronal activity by means of optical spectroscopy. Particular attention will be devoted to the identification and localization of "like" and "dislike" brain centres.

The research will be performed in collaboration with neuroscientists from University of Cagliari (prof. G. Gessa) and CNR dott.G. Colombo). This represents a very interesting opportunity to open a cross research area between physics and neuroscience.. The collaboration will be articulated regarding the specific expertise of physicists and neuroscientist involved.

The research project is scheduled over three years as follows:

1st year:

during the first year the systematic characterization of the fNIR light, diffused by neuronal tissue, will be performed. This issue will allow to distinguish proper scattering mechanisms (Mie, Rayleigh) from other optical processes (fluorescence emission, Raman scattering), thus clarifying the nature of the optical signal related to the neural activity actually still unknown. Moreover other alternative approaches will be evaluated. In particular, the study how coherence properties of the light probe are changed by the interaction with the neural medium will be worth our attention.

2nd year:

based on results gathered during the first year, an experimental protocol will be planned and executed in concern with the neuroscientists of the staff. This part of the research will be focused on: developing the suitable optical setup, identifying the suitable neural tissues; choosing simple neuronal stimulations. This research protocol will be focused on *in vitro* samples.

The results of these experiments will allow to evaluate the sensibility and reliability of the proposed technique, providing a further cross-validation of the results obtained in the first year.

3rd year:

the last year of activity is the most ambitious task of the project: the measurement of the brain activity *in vivo.* Since this conclusive part will be focused on neurobehavioral experiments on living subjects, the neuroscientists of the staff will drive the physicists involved in the measurements and characterizations of the optical signals, in order to avoid artefacts in measuring the brain activity.

The conclusive experiments will be performed on living animals subjected to external stimuli, in order to study and identify the brain activity related to "like" and "dislike" mental states.

In this step the first mandatory task will be to verify that the optical technique previously defined, can be performed in a non-invasive way and they are safe for living subjects. The latter issue is unavoidable from the ethical point of view,

The research team is also involved in the specific research topics of the other members of the OSG (Dr. C.M. Carbonaro, Dr. P.C. Ricci).

UNIVERSITY of CAGLIARI

Department of Physics

1. Research title

Nanomaterials for photonics and sustainable energy

2. Principal investigators

G.Bongiovanni, A.Mura, F.Quochi, M.Saba

3. Research team

Full professors	
Associated professors	G.Bongiovanni, A.Mura
Assistant professors	F.Quochi, M.Saba
Post docs	V.Demontis, C. Figus, D. Marongiu
Ph. D. students	F. Artizzu, M.Aresti, V.Calzia, F.Chen

4. ERC (European Reserach Council) research classification scheme

PE3_12	PE4_3	PE5_4

5. Key words

Nanomaterials	Photonics	*Sustainable energy*

6. National and international collaborations on these topics

C.Simbrunner, H.Sitter, W.Heiss, Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz (A); N.S.Sariciftci, Linz Institute for Organic Solar Cells (LIOS) Physical Chemistry Johannes Kepler University Linz(A); H.-G.Rubahn, Mads Clausen Institute, South Danish University Sonderborg (DK); M.A.Loi, Zernike Institute for Advanced Materials, University of Groningen, Groningen, (NED); H. Yanagi, Nara Institute of Science and Technology (NAIST), Nara (JP); M.V.Kovalenko, D.V.Talapin, Department of Chemistry, University of Chicago, Chicago, USA; A. Mattoni, Istituto Officina dei Materiali del Consiglio Nazionale delle Ricerche (CNR-IOM) Unità SLACS, Monserrato, (IT); C.Cannas, A.Corrias, F.Casula, P.Deplano, M.L.Mercuri, A.Musinu, A.Serpe, Dipartimento di Scienze Chimiche e Geologiche, Monserrato (IT).

7. Abstract

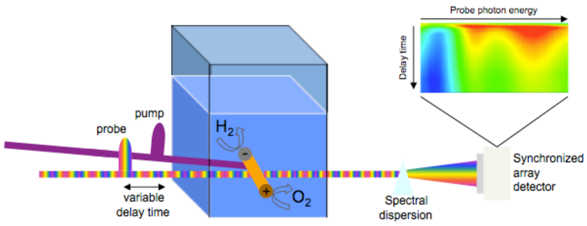
Our objective is the development of novel materials for sustainable energy production and advanced photonic applications. The following research activities are foreseen: (i) design, synthesis, characterization and modeling of semiconductor colloidal nanocrystals for advanced solar cells and low-cost solar fuel production; (ii) design, fabrication and characterization of random nanolasers and surface plasmon lasers; synthesis and characterization of lanthanide complexes for efficient NIR light emission.

8. Framework and state-of-the-art

Colloidal semiconductor nanocrystals and molecular semiconductors are low cost, easy processable materials with tunable and size-controlled optical and electronic properties. Solar energy conversion, energy-saving light sources, quantum information, nanophotonic circuits, bio-imaging are just a few of the applications these materials have been devised for. The planned research activity is addressed to the development of solution-processable nanocrystals for low-cost solar energy conversion, and to the development of novel molecular light sources for optical communications, chemical-sensing and optical imaging.

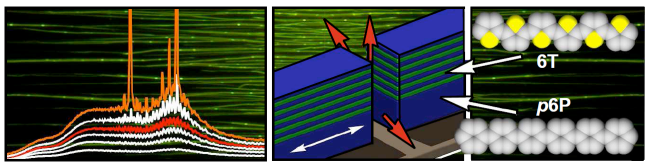
9. Research description, milestones, and goals

The physical phenomena relevant for nanomaterial optoelectronics are optical absorption, charge recombination, separation and vectorial transport. Our experiments will correlate such properties with the morphology and structure of nanomaterials. The results will guide the materials selection and synthesis.

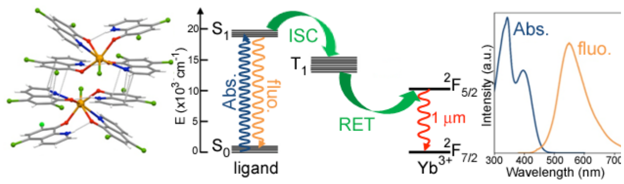


Concerning nanomaterials for harvesting solar energy, our main goal will be to demonstrate heterostructured nanocrystals, produced by solution process, able to efficiently absorb the solar spectrum and to transform the absorbed energy either into electric energy (solar cells) or into chemical energy (solar fuel production and water splitting). We will realize and operate a transient absorption experiment to track the photophysical processes over timescales ranging from picoseconds to milliseconds.

With respect to materials for light emission, we will investigate heterostructured epitaxial nanofibers composed of organic oligomers, as promising materials for nanolasers. Our goal will be to demonstrate low-threshold laser action and lasing with an active volume smaller than the size of optical wavelength. The subwavelength regime will be explored through coupling of optical emission to surface plasmons; we will seek demonstration of the Purcell effect, i.e. a shortening of the radiative decay time of oligomers placed in nanometric proximity to metals supporting surface plasmon modes.



Novel molecular materials will be also designed and tested for infrared optical emission and amplification at telecom wavelengths. Such amplification is currently obtained with Er ions dispersed in optical fibers; compact films with densely-packed Er atoms are plagued by clustering of metal ions and subsequent emission quenching. Our approach will be to assemble a film of organometallic molecules where Er ions are embedded in a molecular cage; molecules will act simultaneously as passivating shell for Er atoms and as an optical antenna, efficiently absorbing visible light and funneling the energy, through Foerster energy transfer, to the emitting metal ion.



1. Research title
Fluorescent silica nanostructure for applications in photonics and biomedecine

2. Principal investigator
Carlo Maria Carbonaro

3. Research team

Assistant Professors	C.M. Carbonaro R. Corpino

4. ERC (European Reserach Council) research classification scheme

PE4_1	PE4_3	PE5_6

5. Key words

Optical spectroscopy	Silica	Nanomaterials

6. National and international collaborations on this topic
Prof. M. Monduzzi, Dr. A. Salis, Dipartimento di Scienze Chimiche e Geologiche, Università di Cagliari
Prof. S. Gerard e Prof. Y. Ouerdane, Laboratoire Hubert Curien (Université de Saint-Etienne)

7. Abstract
The research project aims to investigate silica nanostructures to engineer organic-inorganic hybrids for applications in photonics and biomedicine. The chosen host matrix is mesoporous silica because its huge specific surface area allows to host large concentration of fluorescent organic dye molecules to be exploited as high efficiency emission systems.

8. Framework and state-of-the-art
Mesoporous nanomaterials, whose porosity features are under control, are one of the main topics in design and engineering organic-inorganic hybrids for high-tech applications such as in the field of photonics (dye laser) and biomedicine (fluorescent probes). Mesoporous silica is an ideal matrix to host specific functional molecules (dyes) because of its optical transparency in the visible and near UV range, its thermal and mechanical strength, being also chemically inert and largely biocompatible. The sol-gel synthesis allows to prepare silica nanostructures where the shape, the porosity, the specific surface area and the textural features are under control. The two main drawbacks of the hybrid nanosystems investigated up to now are the leaching of dye molecules and the aggregation phenomena because of the large concentration. The achievement of new mesoporous nanostructures with verified porosity and high efficiency of fluorescence is the aim of the present research, in particular in view of applications as solid sate dye lasers and fluorescent nanoprobes for cell imaging.

9. Research description, milestones, and goals

The framework of the proposed research activity is within the research interests of the Optical Spectroscopy Group (OSG) of the Physics Department where the research team works. The research project goal is to develop fluorescent silica based nanostructure aiming to ascertain the chemical-physical parameters to be controlled and exploited to achieve a very large efficiency of the emission for possible applications in photonics and in the imaging technology for biomedicine. The main concerns are the morphology and the texture of the host matrix in relationship to the host-guest interactions to engineer a multifunctional basic model with different synthesis protocols to achieve ultrafluorescent silica nano- and microparticles to be exploited as solid state dye laser active media or as probes for cell imaging. The specific target is to overcome the two main limitations of the present organic-inorganic hybrid nanosystems: the concentration limit, that is the concentration above which detrimental aggregation phenomena are observed, and the leaching problem, that is the unwanted release of dye molecules depending on the specific external ambient (e.g. polar or non-polar solvents) which reduces the effective dye concentration. In order to hit the mark, we propose to investigate and optimize the synthesis procedure to tailor the morphology and texture of the silica host in view of the enhancement of the fluorescence efficiency. The latter will be pursued by two main actions: the chemical and physical confinement of the dye molecules to avoid the aggregation phenomenon and the grafting of the dye molecules to avoid the leaching problem. A different approach will be also evaluated, by sealing the hybrid micro- and nanoparticles with transparent non porous shell or by specific functionalization of the surface depending on the working ambient (e.g. hydrophobic surface systems to work in water). Finally we propose to bi-functionalize the systems by introducing, beside the dye molecules, metallic nanoparticles to exploit the interaction with plasmons to further enhance the emission efficiency. The research activity is planned for a period of three years and is divided in three work-packages: synthesis, functionalization and characterization of silica based ordered mesoporous materials (OMM) with ordered and controlled porosity; chemical and/or physical immobilization of the dye molecules on the silica surface and characterization of their spectroscopic features; synthesis and characterization of bi-functionalized hybrids. The proposed research is multidisciplinary and will be carried out in close collaboration with the Department of Chemistry and Geology. The project has been recently submitted within the call for research base project of RAS (year 2012) and is under evaluation.

Within the proposed research topic are also included the Visiting Professor project (RE doped silica fibers: fundamental and applicative aspects) which is under the responsibility of the principal investigator and the organization of the international congress “SiO2 Advanced Dielectrics and Related Devices –10th edition” which will be held in Cagliari in June 2014.

The whole staff of OSG (A. Anedda, P.C. Ricci, M. Salis, M. Marceddu) is involved in the proposed research.

The research team is also involved in the specific research topics of the other members of the OSG (A. Anedda, P.C. Ricci, see their proposals for details).

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Magnetic properties of nanomagnets

2. Principal investigator
Giorgio Concas

3. Research team

Full professors	
Associated professors	Giorgio Concas
Assistant professors	
Post docs	
Ph. D. students	Giuseppe Muscas

4. ERC (European Reserach Council) research classification scheme

PE3_12	PE3_11	PE4_2

5. Key words

nanomagnets	nanoparticles	ferrites

6. National and international collaborations on this topic
ISM-CNR, Unity of Montelibretti (RM)

7. Abstract
The objective of this project proposal is the preparation and the study of low dimensional magnetic systems, such as magnetic nanoparticles and molecular magnets.

8. Framework and state-of-the-art
Between the magnetic nanoparticles, relevant nanoparticles are formed by an oxide or by nanocomposites of two different oxides. Among the molecular magnets, we note the multifunctional molecular nanomaterials, constituted by an anionic complex of transition metals (magnetic component) and from an organic molecule (component electrical conductor). The determination of the dependence of the magnetic properties of the structure (size and shape of the nanoparticles and the structure of molecules) is a primary objective of the proposal.

9. Research description, milestones, and goals

The properties will be investigated by DC/AC magnetization measurements with a SQUID-based magnetometer and by studying local magnetic order of Fe by Mössbauer spectroscopy of Fe-57. The study of the properties is complemented by structural characterization. The proponent has extensive years of experience in the characterization of magnetic nanoparticles and molecular materials, in collaboration with researchers of the Chemical Area specialized in the preparation of the same.

Between the magnetic nanoparticles, the nanoparticles of oxides of transition metals (Fe, Co, Ti) are particularly interesting, which couple a ferrimagnetic oxide to one ferroelectric, as the nanostructures ferrite/perovskite. This coupling produces the magnetoelectric effect, which is the induction of magnetization by an electric field or the induction of polarization by a magnetic field. The study of these nanoparticles requires a thorough characterization both after the phase of preparation of the nanoparticles that after any subsequent treatment.

Timing:

a) the preparation and study of nanocrystalline ferrites in the first year;

b) preparation and study of nanocrystalline perovskites in the second year;

c) preparation and study of nanostructures ferrite/perovskite in the third year.

Expected results:

a) determination of the dependence of magnetic parameters on the size and shape of the nanoparticles;

b) determination of the dependence of magnetic parameters on the morphology of nanocomposites;

c) determination of the dependence of magnetic parameters on the structure of molecules.

UNIVERSITY of CAGLIARI

Department of Physics

1. Research title

Nanostructured functional perovskites: emerging phenomena at interfaces and finite size effect on ferroic transitions.

2. Principal investigators

Alessandra Geddo Lehmann and Francesco Congiu

3. Research team

Assistant professors	Francesco Congiu Alessandra Geddo Lehmann

4. ERC (European Reserach Council) research classification scheme

PE3_11	PE5_4	PE5_10

5. Key words

Ferroic transitions	Perovskite oxides	Nanostructured materials

5. National and international collaborations on this topic

Dipartimento di Chimica e Chimica Industriale, University of Genoa
Dipartimento di Fisica, University of Genoa
CNR-SPIN-Naples
CNR-Trieste
CNR-Rome

7. Abstract

Ferroic and multiferroic perovskite-type oxides display attractive properties, including (anti)ferroelectricity, (anti)ferromagnetism, multiferroicity, superconductivity, thermoelectricity and thus exhibit a large variety of functional behavior. Our research will focus on the physical properties of different classes of such complex materials, prepared in the form of nanoparticles and of epitaxial thin films and heterostructures.

8. Framework and state-of-the-art

Although perovskites have been known for a long time, new intriguing physical effects are periodically discovered and their understanding remains an internationally highly competitive area. Hot topics are structural phase transitions, ferroelastics, ferroelectrics, magnetoelectric and in general multiferroic perovskites, lead-free ferroics, new phenomena at perovskite interface. Currently, coupling phenomena in multiferroics and new properties at interfaces in perovskite heterostructures attract the greatest interest. Our research is part of this exciting context. In particular, one of the topics we shall treat, devoted to interface magnetism in perovskite oxides heterostructures, is part of a national project which has just been funded (Prin 2010: Oxide interfaces: new emerging properties, multifunctionalities and devices for electronics and energy storage – OXIDE).

UNIVERSITY of CAGLIARI
Department of Physics

9. Research description, milestones, and goals

The research will be developed along the following three main lines:

Topic 1. Within this topic we shall to address the subject of magnetism at interface between magnetic/magnetic and magnetic/non magnetic perovskite oxides. We shall concentrate on a interfacial coupling effect of great technological impact as well as fundamental interest, i. e. the exchange bias (EB), that we shall study in ferromagnetic (FM) FM/2DEG heterostructures and in FM/ferroelectric (FM/FE) or FM/single phase magnetoelectric bilayers. This topic is part of the PRIN 2010 OXIDE. Therefore a tight collaboration will be established with the experimental partners within that project of CNR-Naples and CNR-Trieste.

Topic 2. This topic will be devoted to the study of the effect of grain size reduction onto the transitions towards magnetically ordered states in perovskites with general formula $RE_{1-x}A_xMnO_3$ (RE=La, rare earth; A=divalent ionic species). We shall investigate in particular the crossover from ferromagnetic to superparamagnetic behavior for RE=La and A=Ca, and the destabilization of the charge ordered states and associated antiferromagnetism in half doped (x=0.5) phase with RE=Pr,Nd,Er,Ho,Yb).

Topic 3*. Within this topic we shall investigate the role that the spontaneous polarization of a ferroelectric crystal may play in improving its photocatalytic activity. The photoconversion efficiency of a semiconductor is, in fact, mainly limited by the recombination of the photogenerated electron-hole couples. Recombination can be drastically reduced in a ferroelectric crystalline particle, because the internal electric field associated to spontaneous polarization can spatially separate charges with opposite sign, driving them to different regions of the particle surface. Our main goal will be to produce, in form of nanoparticles, an innovative ferroelectric photoconverter active in the visible spectral region. To this aim, we shall concentrate on a class of layered perovskites with general formula AnBnO3n+2 (A divalent or trivalent cation and B a mixed valence transition metal), the Curie points of which are the highest among all the known ferroelectric compounds. This highly stable ferroelectric state is likely to be maintained even at the reduced (nanometric) grain size required to maximize the active surface.

Nanoparticles (Topic 2 and Topic 3) will be synthesized by means of soft chemistry techniques. Epitaxial heterostructures (Topic 1) will be produced by PLD and MBE by partners of the PRIN OXIDE. Nanoparticles will be characterized by X-ray powder diffraction, SQUID magnetometry, HRTEM, SEM. Epitaxial heterostructures will be characterized by high resolution X-ray diffraction and SQUID magnetometry.

*Project under evaluation (Regione Autonoma della Sardegna, L.R. 7, Progetti di Ricerca Fondamentale o di base, annualità 2012).

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Study of Porous Silicon for technological applications

2. Principal investigator
Guido MULA

3. Research team

Full professors	
Associated professors	
Assistant professors	Guido Mula
Post docs	
Ph. D. students	

4. ERC (European Research Council) research classification scheme

PE5_6 Porous materials	PE5_8	PE4_1

5. Key words

Porous silicon	Doping	characterization

6. National and international collaborations on this topic
- A. Falqui, R. Ruffilli, Nanochemistry, Istituto Italiano di Tecnologia, Genova
- A. Pezzella, Dip. di Scienze Chimiche, Univ. Federico II di Napoli, Napoli
- M. Mascia, S. Palmas, Dip. di Ingegneria Meccanica, Chimica e dei Materiali, Univ. Cagliari, Cagliari

7. Abstract
In the 2013-2015 years we plan to continue the study of the PSi doping with rare earths and other elements by means of optical, structural and electrochemical characterizations. We also plan to study the potential of porous silicon as a base material for photovoltaic applications by means of impregnating the material using organic molecules.

8. Framework and state-of-the-art Porous Si is a very interesting material for a wide range of applications thanks to several of its properties: high pore's internal surface (up to 900m^2/cm^3), easy tailoring of its formation parameters, fast fabrication process, biocompatibility, … The remarkable internal surface, however, rises several questions without any straightforward answer, first of all the understanding of the chemical reactions at the material surface when organic molecules or inorganic materials are inserted within the pores. Even if the formation processes are well controlled, there is still a lack of understanding of the involved phenomena. Moreover, even when the morphology is essentially the same (like for n^+ and p^+ -type porous silicon) there are significant behavioural differences still unstudied.

UNIVERSITY of CAGLIARI
Department of Physics

9. Research description, milestones, and goals

In the 2012-2015 years we plan to continue our study on the porous silicon formation process and its technological applications. The main research objectives will be:

1) Study of porous silicon impregnated with organic molecules for photovoltaic applications. We plan to test several organic molecules, starting from eumelanin, to improve the spectral range and the photoconversion efficiency of the porous matrix. The main parameters to be studied, beside the chosen molecules, will be the impregnation parameters, the pore size, the contact fabrication procedure. The samples will be characterized by means of electrochemical studies, photocurrent measurements and structural characterization.

2) Study of the impregnation of porous silicon with rare earths and other metals. We plan to improve the knowledge of the electrochemical porous silicon doping process. In particular, we plan to study the formation parameters and mechanisms to improve the samples' homogeneity and optimize the samples' performances. We will consider the behaviour of several elements, starting from rare earths, as a function of the surface properties (e.g. as a function of the oxidation level). The samples will be studied by means of electrochemical measurements, optical spectroscopy, and structural characterization.

3) The phenomena involved in the impregnation/doping of the porous silicon layers are the object of a very few detailed studies, given the complexity of the problem due to the high internal surface of the pores. Among the different techniques that can be used to characterize these processes, galvanostatic electrochemical impedance spectroscopy possess a high sensitivity to the surface properties and is then indicated for porous materials where the internal surface is not directly accessible. For this reason, we will study the porous silicon formation/impregnation/doping processes implying a modification of the surface properties in a combined analysis by means of electrochemical impedance spectroscopy, evolution of the electrochemical processes by their control parameters, optical spectroscopy and structural characterization.

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Phone: **070 675 4703** Fax: **070 510 171** E-mail: **direttore.fisica@dsf.unica.it**

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Optical and structural characterization of nanostructrued semiconductors for optoelectronics applications.

2. Principal investigator
Pier Carlo Ricci

3. Research team

Assistant professors	P.C. Ricci

4. ERC (European Reserach Council) research classification scheme

PE3_12	PE3_1	PE4_1

5. Key words

Nanostructures	Optical Properties	Semiconductors

6 National and international collaborations on this topic
- Prof. A. Rizzi, Physics Department Georg-August University of Göttingen
- Dr. F. Fumagalli and Dr. G. Gulleri, Micron Semiconductor Italia S.R.L.
- Prof S. Ardizzone and Dr. G. Cappelletti, Dipartimento di Fisica Chimica e elettrochimica – Università di Milano.
- Dr. S. Cuesta-Lopez, Advanced Materials - University of Burgos
- Prof. A. Bonfiglio, Dr F. Delogu and S. Palmas – DIEE e DICM, Università di Cagliari

7. Abstract
The Research activity aims to investigate the optical and structural properties of nanostructured semiconductor, i.e. GaN, InGaN, Silicon and organic/inorganic hybrids. The samples will be analyzed starting from their optical and structural properties by optical characterization techniques, mainly: Raman spectroscopy, Steady time and Time resolved luminescence in different temperature conditions.

8. Framework and state-of-the-art
The fundamental research on new semiconductor materials and nanostructured semiconductors is strongly required for the great potential of application in different fields of electronics and optoelectronics. The continuous decrease in the dimensions and spacing of devices on integrated circuits generates secondary and detrimental effects on the nanodimensioned silicon structure, like stress and defects in the dielectric material that fill the nanostructures. The decreased geometrical structures of semiconductors can lead to the fabrication of tunable Light emitting devices with emission in the visible range, in particular it is possible, in principle, to cover the whole visible range by increasing the In concentration in GaN/InGaN/GaN Quantum Well structures (QWs).
Finally, the use of nanostructures hybrid organic / inorganic in electronic devices such as LEDs and FET has become very attractive to increase the versatility of these devices and, simultaneously, reducing their production costs.

9. Research description, milestones, and goals

The framework of the proposed research activity is within the research interests of the Optical Spectroscopy Group (OSG) of the Physics Department where the principal investigator works.

The research activities is divided on three principal field, each of them devoted on the development and the study of new nanostructured semiconductors for electronics and optoelectronics applications. The novelty of the research can be view both on the effects on the principal properties due to the reduced dimensions and on the development on new hybrids materials. The three research projects are planned for a period of three years and can be summarized as:

- Study on the stress effects and defects on Silicon nanostructures.
- Optical and structural properties of field effect organic biosensor.
- Emission properties of GaN-BASED hetero- Nanostructures.

The first project, in collaboration with the Micron Semiconductors Inc., consists in the study of Silicon wafers by Raman spectroscopy and luminescence measurements. The first mentioned experimental technique will be utilized to study stress effects as a function of the growth parameters and dimension of flat wafer in Silicon nanostructures. Luminescence and time resolved luminescence measurements will be carried out to identify and study the defects (surface or bulk) on the dielectrics materials that cover the wafers and fill the nanostructures.

The study of the optical and structural properties of field effect organic biosensor, carried out in strict collaboration with DIEE and DICM departments of the University of Cagliari and the Chemistry Department of the University of Sassari, was financed by the Regione Autonoma della Sardegna (RAS) within the “BIOFET” project (code CRP -27388). The project fits the organic electronics development, more specifically for sensors based on organic semiconductors and aims to study from different scientific points of view, the interfaces that constitute a field effect device. More specifically, the study will be performed by optical methods (Raman and luminescence spectroscopy) on the covering bio layer of electrodes: information on bonding, thickness, density and defects will be utilized to the development of new hybrids device.

Finally the third research project is in the field of semiconductor nanostructures based on the GaN material system and related alloys – InGaN and AlGaN. In particular we are interested in the optical properties of bottom-up fabricated semiconductor nanowires (NWs) and nanocolumns (NCs). More precisely, we want to tackle this issue by a quantitative comparison of photoluminescence quantum efficiency in Quantum Well structures grown by Molecular Beam Epitaxy in 2D- as well as in columnar nanostructures. The project will be carried out in close collaboration with the Faculty of Physics of the Georg-August University of Göttingen. Within the proposed research topic is also included the Visiting Professor project (Optical and structural properties of GaN-based hetero- nanostructures) which is under the responsibility of the principal investigator.

The whole staff of OSG (A. Anedda, C.M. Carbonaro, R. Corpino, M. Salis, M. Marceddu) is involved in the proposed research.

The research team is also involved in the specific research topics of the other members of the OSG (A. Anedda, C.M. Carbonaro, see their proposals for details).

UNIVERSITY of CAGLIARI
Department of Physics

RESEARCH PLAN

Domain "Condensed matter physics"

Sub-domain 02B2 "Theoretical condensed matter physics"

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
High -T_c superconductors: a first principles investigation.

2. Principal investigator
Fabio Bernardini

3. Research team

Full professors	Sandro Massidda
Associated professors	
Assistant professors	Fabio Bernardini
Post docs	Marco Monni
Ph. D. students	

4. ERC (European Reserach Council) research classification scheme

PE 3_8		

5. Key words

Electronic properties	Superconductivity	Magnetism

6. National and international collaborations on this topic
Halle, Max Planck Institute (Prof. E. K. U. Gross)
Università di Parma (Prof. R. De Renzi)
Università di Genova (Prof.ssa M. Putti)
Università di L'Aquila (Dott. G. Profeta, Prof.ssa A. Continenza)

7. Abstract
We will study high-Tc superconducting materials based on iron. Our computational investigation based on DFT will focus on the relationship between magnetism and superconductivity. We will work on experimental data of magnetoresistance and µSR made available by our experimental partners.

8. Framework and state-of-the-art
We will study the superconductivity in iron-pnictides, a class of superconductors discovered in 2008, where Tc reaches 55 K. These materials are important because they are an example of high-temperature superconductors whose electron correlation does not make impossible a first principles investigation of their electronic properties by DFT. It is assumed that the mechanism of superconductivity is mediated by interactions of the magnetic type. It is therefore important to investigate the relationship between magnetism and superconductivity in these materials.

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9. Research description, milestones, and goals

The purpose of the research that we will carry on over the next three years is the study of the relationship between magnetism and superconductivity in high Tc superconductors. Our investigation will focus on iron-pnictides although the discovery of new materials could extend our investigation. Thanks to the collaboration with experimental partners in Genoa (Prof. M. Putti) and Parma (Prof. R. De Renzi) we will have available experimental data on the magnetic properties of compounds such as iron-pnictides of the class 1111 (REFeAsO, RE = La, Ce, Pr, Sm) 122 (BaFe2As2) and 11 (FeTe, FeSe). They are essentially data of magnetoresistance, Hall effect, resistivity whose interpretation is at the basis of the understanding of the band structure in these materials. In particular, we are interested in studying how the appearance / disappearance of the magnetic phase affects the band structure and the topology of the Fermi surface.

These data will be complemented with the study of magnetism at the microscopic level using the muon spin rotation (μSR) technique. μSR allows the investigation at the microscopic level of the intensity of the magnetic fields perceived by a muon in the interstitial region of a solid. The interpretation of these data is less direct than that given by Mössbauer spectroscopy and requires the identification of the muon localization site. So this is a typical technique where collaboration between theoretical and computational investigation based on DFT and experimental investigation complement well. Then we will study the microscopic magnetic properties of iron-pnictides already mentioned comparing them with the experimental data. This second part of our activity will not be limited only to iron-pnictides since the technique is quite general and allows us to study any magnetic material or not. In both investigations, we will make use of existing collaborations with the groups of l'Aquila and the Max-Planck Institute in Halle, given their experience in the theoretical study of superconductivity in iron-pnictides and in the study of magnetic materials. Moreover, in collaboration with the Max-Planck Institute in Halle we will test a new method for predicting new superconductors based on the combined use of the SCDFT approach and a search algorithm based on the minimal hopping method.

We expect that our project will be divided in three years with the following schedule essentially based on the material to be studied:

2013 – Investigation of iron-pnictides class 11 i.e. FeTe e FeSe

2014 – Investigation of transport properties of iron-pnictides class 1111 i.e REFeAsO (RE=La,Ce,Pr,Sm)

2015 – Investigation of magnetism in $BaFe_2As_2$, and $CaFe_2As_2$ as a function of doping. Study of new superconductors suggested through the search by the minimal hopping method.

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UNIVERSITY of CAGLIARI

Department of Physics

1. Research title

Electronic and optical properties of materials

2. Principal investigator

Prof. Giancarlo Cappellini

3. Research team

Full professors	
Associated professors	Giancarlo Cappellini
Assistant professors	
Post docs	A post-doc to be hired early 2013
Ph. D. students	

4. ERC (European Reserach Council) research classification scheme

PE3_5	PE3_7	PE2_8

5. Key words

Solid State Physics	Spectroscopy	Applied Physics in Medicine

6. National and international collaborations on this topic

Dr.ssa Maurizia Palummo, Dipartimento di Fisica, II Università di Roma ''TorVergata''
Dr. G. Mulas, OAC-INAF, Cagliari, Italy
Prof.F. Bechstedt, Direttore IFTO- FSU Jena ,Germany
Prof.Fabio Finocchi, INSP, UPMC Université Paris 06, CNRS, France
Prof.Lucia Reining, Ecole Polytechnique, Palaiseau, France

7. Abstract

The proposed project will deal with the electronic and optical properties of the following systems:
A) Large gap crystals : the case of the fluorides,
B) PAHs molecules.
These issues will be treated within computational simulation techniques.

8. Framework and state-of-the-art

The spectroscopic techniques have played a fundamental role in the study of the electronic and optical properties of solids, molecules and atoms. The results after those techniques have permitted the experimental confirmation of theoretical models relative to atomic and molecular structures during the period of the first successes of the quantum theory of matter. With respect to solid state physics afterwards the optical absoprtion spectra, the energy loss spectra and the surface reflectivity measurements turned out to be of fundamental importance for the understanding of the electronic structure of those materials which play a role in optoelectronics applications. The above scenario has been modified by the introduction of new computational codes, named ab-initio ones, for the calculation of the electronic properties of localized and extended systems. Those parameter-free codes have permitted the accurate calculation of electronic transitions in solids and molecules of different nature and symmetry. The use of the above techniques of theoretical spectroscopy will be main goal of the present research plan.

9. Research description, milestones, and goals

The parameter-free computational codes devoted to the calculation of the spectroscopic properties of materials can be of different kind: DFT-LDA ones(based on density functional theory within the local density approximation for the exchange and correlation energy) or DFT-GW ones for the calculation of self-energy effects in the GW apporximation), TD-DFT ones (in which the time evolution of the electronic density is considered) or BSE ones (in which the Bethe-Salpeter equation is used to treat the electron-hole interaction). More info about techniques, their origin, the comparison with experimental results could be found at the web site of ETSF network http://www.etsf.eu. The European Theoretical Spectroscopy Facility (ETSF) is a network of more than 200 high-level researchers .The research program we shall tackle will be performed in collaboration with ETSF colleagues and consists of the following parts:

A) Electronic and optical properties of large band-gap systems: the case of fluorides

Large band-gap materials are very promising materials for possible application in modern optics and in optoelectronics. Ionic crystals with the fluorite structure for example show large band-gap and high transparency in a wide-frequency range. For ground-state calculation (lattice parameter, bulk modulus, total energy) DFT-LDA codes will be used. We will deal then with the one-particle excitations: for this issue we shall use the GW approximation for the electronic self-energy operator. A deep comparison with respect to experimental results and to other theoretical ones will then follow. For the fluorites under study we shall turn then to the calculation of the dielectric function in different approximations (RPA, GW).

In the following part of the project we shall study the possibility to include the electron-hole interaction in the optical absorption spectrum. We have in schedule to perform simulations within the Bethe-Salpeter (BSE) scheme.

B)Electronic and optical properties of PAHs

The use of the above mentioned computational techniques had a strategc importance in the last years fo the calculation of the electronic and optical properties of molecules of interest for astrophysics and astrochemistry. Between the molecular species interesting in the astrochemistry field the large molecules of carbonaceous basis are of fundamental importance; in particular the polycyclic aromatic hydrocarbons (PAHs) and their derivaties which should be one of the most abundant families in space. Some of these molecules are of importance for possible optoelectronic applications when considered in their solid phase. Therefore is evident the importance of the present study with respect both to the fields of materials science and astrochemistry.Between the possible results we forecast the following ones. Study of the homologous PAHs families and their derivaties, fullerenes, Carbon based nanostructures. Study of ground state properties.Quasiparticle properties determined within Δ-SCF method. Optical absorption properties after different techniques: whole spectrum study up to extreme UV within a TD-DFT scheme in real time and space on one side and on the other hand study in the onset region of the separated contributions involved in each transition using a frequency space TD-DFT method. If possible comparison between the obtained results and data obtained within GW and/or BSE schemes. Charged and neutral systems, differences in the optical and electronic properties .

UNIVERSITY of CAGLIARI

Department of Physics

1. Research title

Efficiency of localized-orbital methods in computational solid state

2. Principal investigator

Francesco Casula

3. Research team

Full professors	Francesco Casula
Associated professors	
Assistant professors	
Post docs	
Ph. D. students	

4. ERC (European Reserach Council) research classification scheme

PE3_5	PE3_12	

5. Key words

Computational physics	Localized functions	clusters

6. National and international collaborations on this topic

7. Abstract

Comparison of results obtained by means of simlified localized-orbital methods in order to verify the advantages of their use in solid state computations.

8. Framework and state-of-the-art

9. Research description, milestones, and goals

Solid. state and cluster computation percome by state-of-theart methods compared with our localized funcion results in order to prove their efficiency in extensive stuies crystal e cluster properties.

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UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Theory and simulations of nanomaterials

2. Principal investigator
Luciano Colombo

3. Research team

Full professors	Luciano Colombo
Associated professors	
Assistant professors	Claudio Melis
Post docs	a post-doc to be hired early 2013
Ph. D. students	Claudia Caddeo Fabio Manca Maria Ilenia Saba

4. ERC (European Reserach Council) research classification scheme

PE3_12	PE3_17	PE5_10

5. Key words

Energy materials	Nano-/bio-mechanics	Atomistic simulations

6. National and international collaborations on this topic
- University of Genova, Modena, Padova, Roma "La Sapienza", Trieste, Politecnico di Milano , and SISSA (project PRIN-GRAF); University of Milano (project ELDABI)
- National Research Council (CNR): IOM, IMM, and SPIN institutes
- Institut d'Electronique, Microelectronique et Nanotechnologie, Université de Lille (F)
- Institut de Ciència de Materials de Barcelona (ICMAB-CSIC)

7. Abstract
We are interested in understanding the physical behavior of novel nanomaterials for nanoelectronics, optoelectronics, energy production/harvesting (photovoltaics or co-generation for green electronics), nanomechanics, and medical applications. We focus on theoretical and computational modeling by concurrent combinations of statistical mechanics, materials physics, atomistic simulations, and continuum elasticity.

8. Framework and state-of-the-art
Environment-friendly energy production, energy-efficient technologies, and bio-compatible materials are main concerns in our society, as outlined in the *"Horizon 2020*" EU document, focused on the search for new energy supplies, the design of more energy-efficient equipments, and the development of nanomaterials for biomedical devices . In particular, it is possible to conceive a *materials-by-design* approach where natural materials are manipulated at the nanoscale, resulting into new tailored systems meeting application-specific needs. In this framework atomistic simulations are playing an increasingly important role and our research will be addressed to improving the basic understanding of the physical behavior of nanomaterials as much diverse as: graphene, SiGe thermoelectrics, nanocrystalline silicon, dielectric elastomers, and (model) biopolymers.

9. Research description, milestones, and goals

Keyword ENERGY - By means of all-atom large-scale molecular dynamics (MD) simulations, we will work on the following perspectives of paramount relevance for nano-technology:

- hybrid organic/inorganic nanomaterials for photovoltaics: predictive theoretical modeling of photophysics in polymer/inorganic interfaces, aimed at a novel class of materials with improved photoconversion efficiency;
- nanocrystalline silicon for optoelectronics and photovoltaics: predictive theoretical modeling of quantum confinement effects in nanocrystalline silicon as a promising material for oxygen-free optoelectronics, silicon-based memories and photovoltaics;
- nanoscale thermal transport: predictive theoretical modeling of heat flux in nano-systems, including SiGe bulk nanostructure (as high-efficient thermoelectrics) and graphene nanoribbons (as heat sinks for optimal thermal budget of ULSI devices).

Part of this activity will be supported by PRIN 2010-2011 project "GRAF".

Keyword NANO-/BIO-MECHANICS - The main focus will be on the combined application of atomistic simulations (at MD or Monte Carlo level) and elasticity theory to the determination of the effective elastic/mechanical properties (both linear and non-linear) of nanocomposite materials, two-dimensional atomic sheets, as well as model polymer chains of biological/biomedical interest. In particular, we will address the following topics:

- graphene-based systems: blended continuum/atomistic description of linear and nonlinear elastic moduli (corresponding to either stretching and bending deformations) of both pristine and defected graphene, as well as of its stoichiometric/non-stoichiometric hydrogenated conformers (graphane);
- model polymer chains of biological interest: statistical mechanics investigation on the finite-size elasticity of two-state biopolymers in both the constant-force (Gibbs) and constant-displacement (Helmholtz) ensemble. Theoretical calculation of the prototypical force-extension curves for short and long chain polymers and search for a universal model;
- dielectric elastomers: large-scale atomistic simulation of the impact of metal clusters on polydimethylsiloxane (PDMS) films as function of implantation parameters and physico-chemical characteristics of the substrate (entangled melt vs. cross-linked polymer chains). Determination of the microstructure evolution of the post-implanted film (induced surface roughness and swelling, formation of nanopores, gathering of implanted clusters and formation of buried metallic wires). Resulting electro-mechanical behavior of implanted PDMS;
- nanostructured materials: multiscale modeling of linear and nonlinear elastic features of nanocomposites, nano-grained materials, and graded interfaces, as well as on the mechanical failure in multi-cracked systems.

Part of this activity will be supported by projects ELDABI and ISCRA "UCIP".

Keyword ATOMISTIC SIMULATIONS - We will sustain a continuous effort toward developing increasingly-efficient and scalable codes for large-scale atomistic simulations in materials physics. In particular, especially computer-intensive applications will be made possible by new achievements such as:

- low-complexity algorithms (order-N or divide-and-conquer methods for quantum calculations);
- acceleration techniques for long time scale MD simulations;
- algorithms for efficient particle labeling.

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Ordering, transport, magnetism in correlated systems: theory and applications

2. Principal investigator
Vincenzo Fiorentini

3. Research team

Full professors	
Associated professors	Vincenzo Fiorentini
Assistant professors	
Post docs	
Ph. D. students	Francesco Ricci

4. ERC (European Reserach Council) research classification scheme

PE3_5	PE3_11	PE3_12

5. Key words

Ab initio theory	Multiferroicity	Magnetism

6. National and international collaborations
- CNR-ISC Roma: new density-functionals for correlated systems
- CNR-ISM Roma: spintronics materials
- Università di Liegi: electronic transport in low-dimensional systems
- Trinity College Dublin: theoretical methods for correlated materials
- CNR-SPIN Genova: oxide interfaces and thin film growth

7. Abstract
We will further the development and application of advanced ab initio methods to nanostructured systems with magnetic, orbital, charge, etc. order where conventional methods fail. Our applicative goals are non-conventional multiferroics and hybrid FE-FM interface nanosystems for resistive switching applications. We also cultivate collaborations on e.g. electronic structure and transport at oxide interfaces and on diluted-magnetic spintronic materials. Among our mid-term goals, we plan to branch out into the physics of f-shell systems, which are relevant for e.g. nuclear waste management applications.

8. Framework and state-of-the-art
Our activity is at the crossroads of advanced ab initio theory and of visionary device concepts for future all-oxide electronics. Even aside from the great basic interest and value, we envisage intriguing applications such as, e.g., high-density multistate memories and spin-selective electronics building blocks (spin-valves, etc.).

9. Research description, milestones, and goals

We employ methods ranging from conventional (LDA, GGA) to advanced (hybrid, SIC), besides our own version of transport Bloch-Boltzmann theory and the occasional magnetism models based on ab initio quantities. This enables us, whenever necessary, to tackle systems and materials resisting conventional approaches. Our activities for 2013 are now summarized.

Non-conventional multiferroics

We will extend the study of magnetic doping of the topological ferroelectric $LaTiO_{3.5}$ to other dopants producing ferromagnetism (FM). We will compute virational magnetoelectric coefficients in a few promising cases (LTO:Mn, LTO:Fe). We expect to have some of these studies appear within 2013.

Hybrid FE/FM interface nanosystems

We started the study of the depolarizing field and of spin-polarized charge accumulation and depletion at the interfaces of ferroelectrics ($PbTiO_3$) and magnetic metals ($SrRuO_3$, Co). We plan to use selectively and locally V-doped PTO (which appears to be FM) to help drive the interface charge and the internal field, with a view to applications e.g. to spin-valves or magnetically-driven spin-selective resistive switching. PTO:V and the undoped interface will certainly be done by end 2013.

Electronic structure of oxide interfaces

We are extending of our earlier work on the classic $SrTiO_3/LaAlO_3$ system to buttress our previous identification of the localization mechanism producing the 2DEG at insulating-oxide interfaces with the correlated nature of (nearly-)singly-occupied 3d Ti orbitals. Specifically we are studying Nb-δ-doped STO as well as the $SrZrO_3/SrTiO_3$ and $SrSnO_3/SrTiO_3$ interfaces. A couple of these papers should be out by end 2013.

Diluted-impurity magnetism in oxides

We are out to pinpoint the mechanism of FM in Cr-doped In_2O_3 and Sn:In_2O_3 (ITO). Our preliminary work suggests that previous interpretations are wrong, and that Cr cannot sustain FM. We surmise that defects, most likely native, are the key to activating Cr FM. The interest in this topic is obvious, given the ubiquity of ITO in opto- and nanoelectronics. The Cr:ITO work will be certainly over in 2013, and the native-defect/Cr work may be at an advanced stage.

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Computational studies of systems of biological and pharmacological interest

2. Principal investigator
Paolo Ruggerone

3. Research team

Full professors	
Associated professors	Matteo Ceccarelli Paolo Ruggerone
Assistant professors	
Post docs	Attilio V. Vargiu
Ph. D. students	Pierpaolo Cacciotto, Daniela Fadda

4. ERC (European Reserach Council) research classification scheme

PE3_19	LS2_11	PE4_13

5. Key words

Bacterial resistance	Proteins	Computer simulations

6. National and international collaborations on this topic
- Jacobs University, Brema (Germania)
- University of Berkeley, Berkeley (USA)
- University of St. Andrews, St. Andrews (UK)
- Karlsruher Institut für Technologie, Karlsruhe (Germania)
- King's College, Londra (UK)

7. Abstract
In the next years we will focus our attention on the study of transport properties of compounds through membranes of both bacteria and mitochondrial cells within the framework of IMI and PRIN-2010 projects. Additionally, we will continue the research on oxygenases (enzymes that oxidize a substrate) and on twin arginine translocation systems (Tats), which transport proteins through cell and bacteria membranes.

8. Framework and state-of-the-art
As mentioned above, our research on some of the resistance mechanisms developed by bacteria is timely and appropriate, as demonstrated by the recently approved IMI project of the European Community. Indeed, bacterial antibiotic resistance appears no more as a threat but is a real emergence according to health. To gain possible general insights into transport properties through membranes we will study the translocation of molecules through mitochondrial membranes within the framework of an approved PRIN-2010 project. The two other main research projects on oxygenases and Tats are well inserted in ongoing international collaborations. They are complex and sophisticated protein systems involved in the catalysis of processes (oxygenases) and in the transport of functional proteins through

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cellular and bacterial membranes. Publications in high-impact journals are in press (Cell, Tats) or in preparation (oxygenases).

9. Research description, milestones, and goals

Our methods are computational and range among different degrees of accuracy, from quantum chemistry (QM) approaches to classical molecular dynamics (MD) simulations including state-of-the-art methods of free energy sampling, from kinetic Monte Carlo (KMC) method to docking and bioinformatics programs. We sketch the main points of our researches as follows:

<u>Bacterial resistance</u>

a) Study of antibiotic translocation through bacterial pores and of antibiotic extrusion by efflux systems (classical MD, QM, Metadynamics, Steered MD, Targeted MD) (2013-2015);
b) Docking and bioinformatics programs used to identify possible binding sites of compounds in pores and efflux pumps and to compensate the lack of structural data concerning the spatial arrangements of the protein under investigation (Attract, Autodock, Modeler, BLAST) (2013-2015);
c) KMC simulations to evaluate kinetics parameters associated with the translocation and extrusion processes in bacteria. These simulations will rely on the outcomes of the studies described in items a) and b) (2014-2015).

<u>Permeability of the mitochondrial membrane</u>

a) Study of the transport of molecules through VDAC, a protein of the mitochondrial membrane (MD and Metadynamics);
b) Study of the gating mechanism in the VDAC protein (Metadynamics).

<u>Oxygenases</u>

a) Study of the diffusion of oxygen and water molecules inside the protein and comparison with electronic density maps from X-ray experiments (classical MD and Metadynamics).

<u>Twin arginine translocation systems</u>

a) Study of the possible equilibrium configurations of the different Tats components. By combining these components allow the passage of functional proteins through cellular and bacterial membranes without producing leakage. Identification of the relevant interactions and of the residues crucial for the stability and functioning of the system (classical MD) (2013-2014);
b) Study of assembling process of the different Tats components. Identification of the bottleneck steps during the process (Metadynamics) (2014-2015).

UNIVERSITY of CAGLIARI
Department of Physics

RESEARCH PLAN

Domain "Condensed matter physics"

Sub-domain 02B3 "Applied physics"

UNIVERSITY of CAGLIARI
Department of Physics

1. Title of the research line
Study of the implementation of diagnosis and advanced therapies in cancer, neuropathy, cardiology

2. Responsible
Mario Caria

3. Participants

Professori ordinari	
Professori associati	
Ricercatori TI e TD	Mario Caria
Assegnisti di ricerca	
Dottorandi	

4. ERC (European Reserach Council) research classification scheme

LS7_1 Medical engineering and technology	LS7_2 Diagnostic tools	LS7_10 Public health and epidemiology

5. Parole chiave

Electrophysiology	Cancer resaerch	

6. National or international collaboration on this specific research

7. Summary
We intend to study the implementation of innovative procedures in the diagnosis and treatment of cancer, cardiology and neuropathy in hospitals. We want to compare the Health Technology Assessment in different countries and predict the development of innovative diagnostic and therapeutic techniques and clinical pilot studies to lead to appropriate DRG.

8. General framework
Currently, a number of HTA systems are in use worldwide. Their implementation varies from country to country and in Italy for macro regions. Several national and international organizations are meant to oversee better implementation but they differ in the judging criteria. The study is meant to check for various diseases ranging from breast cancer to the bladder or non-invasive diagnosis of angina until the peripheral neuropathy, how an HTA can adapt to new technical proposals. This is done through the analysis of the pivotal clinical studies aimed at verifying HTA and the time and manner of allocation of appropriate DRG.

9. Description of the research, timing and expected results

In order to check for different conditions ranging from breast cancer to that of the bladder or the non-invasive diagnosis of angina through the peripheral neuropathy, on how the HTA can adapt to new techniques proposed, it is performed an analysis of clinical pilot studies to verify the HTA as well as when and how to assign appropriate DRG.

It is expected to analyze first new therapies for the treatment of metastatic or at least several cancers among the most common ones (breast, lung, skin, etc. ..). For this sake the occurrence of clinical pilot studies in eg innovative therapies including immunotherapies are associated to the corresponding diagnosis for both imaging techniques that of in vitro testing.

We study the possibility and possible implementation of ad hoc tests associated with the therapy and a possible DRG on an international scale.

This phase is expected in about six months, the time necessary for the performance of the activity.

The expected results are evidence of a possible DRG on an international scale.

For cancer or other pathologies of the reproductive apparatus we will analyze the status of delivery systems with or without electrical stimulation and drugs associated and how their dosages and times must be adjusted to the DRG in force.

We will analyze the diagnosis and treatment in the field of neuropathic with particular reference to electrophysiology. We will analyze the progress made on achieving DRG specific geographic areas.

This phase is expected to last six months, the time necessary for the performance of the activity.

The expected results are evidence of DRG specific geographic areas.

The field of non-invasive cardiology will be analyzed from the point of view of the new remote monitoring solutions and the impact on new procedures for their HTA. To this effect an analysis of the possibilities offered by the new ACO in the U.S. and how these will impact on HTA in all areas where the EHR are possible for specific pathology is done. In the case of patients with heart disease it will be validated how the change will occur in its management and its benefits and if these lead to a correction of the HTA.

This phase is expected to last about six months, the time necessary for the performance of the activity.

The expected results are evidence of a correction of the HTA.

UNIVERSITY of CAGLIARI

Department of Physics

1. Research title

Physics applied to medicine, art, and environment

2. Principal investigator

Paolo Randaccio

3. Research team

Associated professors	Paolo Randaccio
Assistant professors	Viviana Fanti, Loredana Satta
Students of the Specialization School in Medical Physics	Alessandra Bernardini Gianluca Daddii Valentina Del Rio Walter Flore Marco Serra

4. ERC (European Reserach Council) research classification scheme

PE2_16 Metrology and measurement	LS7_8 Radiation therapy	LS7_2 Diagnostic tools (e.g. genetic, imaging)

5. Key words

Ionizing radiation dosimetry	Archaeometry	Radiotherapy and Nuclear Medicine

6. National and international collaborations on this topic

Within the project PRIN 2010-2011 entitled: "Development and application of new materials for ionizing radiation dosimetry", collaboration with the research units of: Pisa, Milan, Pavia, Palermo, Turin.

7. Abstract

The research is divided into several sub-projects:
1. Development and application of new dosimetric techniques (PRIN)
2. Techniques for dating of archaeological finds
3. Dosimetric study in the Department of Neonatal Intensive Care
4. Individualized dose calculation in nuclear medicine therapy.

8. Framework and state-of-the-art

1. In modern radiotherapy the spatial distributions of dose is so complex that it requires the development of versatile three-dimensional dosimeters, convenient for clinical use and with the accuracy and resolution necessary to enable comprehensive verification of complex dose distributions.
2. The ceramics contain crystals of silica and feldspar exhibiting the phenomenon of thermoluminescence. The ceramic finds buried for long periods are subject to radiation due to natural radioisotopes present in the soil, as a result the crystals absorb such a dose that can be measured using the thermoluminescence.

3. The radiosensitivity of children is known to be equal to three times that of adults. Hence the need to assess the dose and the risk of cancer in children, linked to numerous radiological investigations that are carried out in premature infants.
4. In nuclear medicine therapy, the administered activity is determined on the basis of standard protocols without taking into account the characteristics of individual patients. The present work arises from the need to evaluate and optimize the individual dose absorbed by the target organ in order to make the therapeutic treatment more effective, but at the same time restrict the dose to other organs and tissues.

9. Research description, milestones, and goals

1. The activity is focused on the reconstruction of tomographic sections from linear optical scans. We will construct a scanning system consisting of two distinct apparatuses: the first for the rotation of the cylindrical phantom around its axis, the second for the translational motion in two dimensions of the laser beam and of the reading system. Furthermore, we intend to characterize the dosimeters based on OSLD detectors, used in radiology, and also known as phosphor plates.
2. Our group has started an activity in the field of Archaeometry in collaboration with the Department of Archaeology, University of Cagliari using instrumentation and knowledge developed in the field of environmental radioactivity and radiation dosimetry. The project is still in its infancy and has resulted so far in a thesis, a postgraduate Master's thesis and presentations in local congresses.
3. The purpose of this sub-project is to obtain a correct evaluation of the dose and risk, in order to optimize the absorbed dose. A comparison with the European guidelines on quality criteria for pediatric diagnostic radiology (EUR16261) will be also carried out. From the experimental point of view, we will execute the direct measurements of ESD (Entrance Skin Dose) in vivo and in anthropomorphic phantoms, using different methods of measurement: TLD (Thermo Luminescence Dosimeter), DAP (Dose Area Product) with a transmission ionisation chamber, OSLD (Optically Stimulated Luminescence Dosimeters), gafchromic films. The study with OSLD has a direct link to the sub-project 1. For the estimation of the effective and equivalent doses to the organs of the patient, a Monte Carlo-based software (PCXMC) will be used.
4. In order to achieve the optimization of individual dose, we will first proceed to quantify the distribution of activity through characterization of nuclear medicine equipment such as: SPECT-CT and PET, through the use of specific phantoms; then the comparison between different methods of calculation such as: MIRD, OLINDA and Monte Carlo codes will be made.

UNIVERSITY of CAGLIARI
Department of Physics

RESEARCH PLAN

Domain "Astronomy, astrophysics, and physics of earth and planets"

Sub-domain 02C1 "Astronomy, astrophysics, and physics of earth and planets"

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Observational and Theoretical Study of X-Ray Binaries and Neutron Stars

2. Principal investigator
Luciano Burderi

3. Research team

Full professors	Nicolò D'Amico
Associated professors	Luciano Burderi
Assistant professors	Alessandro Riggio
Post docs	
Ph. D. students	

4. ERC (European Reserach Council) research classification scheme

PE9_10	PE9_11	PE9_13

5. Key words
inserire al massimo 3 parole-chiave a scelta libera

High Energy Astrophysics	Radioastronomy	Pulsar

6. National and international collaborations on this topic
Dipartimento di Fisica, Università di Palermo
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7. Abstract
The main topics of our research are High Energy Astrophysics and Radioastronomy, in particular, the study of binary systems containing a compact object (very weakly magnetized neutron star or black hole) and Radio Pulsars. The research conducted in this field is mainly based on observations obtained with instruments placed on board satellites for X-ray astronomy and observations in the Radio and Gamma bands.

8. Framework and state-of-the-art
Low-Mass X-ray Binaries (LMXBs) consist of a neutron star (NS), with weak magnetic field ($<10^{10}$ Gauss), accreting matter from a low-mass (<1 Msun) companion. Most of these systems are X-ray transients usually found in a quiescent state, with luminosities in the range 10^{31} -10^{33} ergs/s. On occasions they exhibit outbursts, with peak luminosities between 10^{36} and 10^{38} ergs/s. The inferred variations in the mass accretion rate are typically a factor of 10^{5}. LMXBs are related to Millisecond Radio Pulsars (MSPs) a class of about 200 radio pulsars with spin period shorter than 10 milliseconds. It is believed that MSPs are old NS, spun-up to millisecond periods by a previous phase of accretion of matter (and angular momentum) in a LMXB. This is the so-called Recycling Scenario.

9. Research description, milestones, and goals

Our Unit includes researchers with great experience in observations in all the bands of interest (X-ray, radio, optical, gamma), as well as experts in binary evolution. In particular we plan to perform: 1) Timing analysis of several X-ray outburst of AMSs to constrain the orbital and spin parameters and to follow, through the study of subsequent outbursts, their secular evolution. 2) X-ray spectral analysis of AMSs in order to constrain the geometry and properties of the emitting region. 3) Optical observations of AMSs in outburst and, most important, in quiescence, when accretion luminosity is over and the albeit elusive power emitted by the rotating magnetic dipole is reprocessed by the companion (acting as a bolometer) in the optical band. 4) Radio observations of AMSs in quiescence in the hope of detecting coherent radio pulsations which, although thoroughly searched, are still missing from these sources. Our present understanding of these systems indicates that observations at several GHz offer the most promising opportunity to detect pulsations in radio. 5) Hard and soft gamma-ray observations of AMSs in which folding techniques with the extremely accurate parameters derived in a) could lead to the first detection of AMSs in the gamma-ray band. 6) Theoretical modelling of LMXBs, AMSs, and MSPs evolution. In this field we will explore the role of the radiation pressure of the magneto-dipole emission and the spin-down torque associated with it, which has been neglected in most of the evolutionary scenarios proposed up to date. 7) Timing analysis of MSPs. We plan to continue on applying state-of-art timing procedures to the best available pulsar for studies of gravity theories, namely the Double Pulsar. This will lead to unprecedented tests of general relativity and possibly constraining the equation of state for the nuclear matter. 8) Detection of Gravitational Waves. Within the context of the European Pulsar Timing Array (EPTA) collaboration, we will be deeply involved in an unprecedented experiment, that aims to combine the capabilities of the major european radio telescopes. This will allow us to achieve a very high accuracy in the determination of the times of arrival of the radio pulses from the targeted MSPs, thus paving the way to a direct detection of the cosmological background of gravitational waves. 9) The EPTA radio telescopes will also be used for performing multi-wavelength observations of a large sample of eclipsing MSPs. They play a key role in the investigation of the last stages of the evolution of the MSPs and in particular in the formation of the isolated MSPs. 10) Within the context of the High Time Resolution Universe (HTRU) collaboration, we will carry on an ultra-deep search for additional MSPs at the Parkes radio telescope. Some of the new MSPs will be suitable for a Pulsar Timing Array, or as laboratories of gravity theories, or for studies of the formation of the isolated MSPs or, more in general, for investigating the evolutionary link between AMSs and MSPs .11) The Agile and Fermi databases will be also exploited to fully characterize the phenomenology of the radio-loud gamma-ray pulsars, in order (i) to shed additional light on the still debated electrodynamics of the rotational powered neutron stars, and (ii) to identify peculiar pulsars with transitional physical properties with respect to other classes of neutron stars. 12) We will perform an observational program (from the radio to the gamma-ray band) to properly measure the spatially-resolved spectra of Supernova Remnants and Pulsar Wind Nebulae to discriminate between leptonic and hadronic models for high energy emission from these structures.

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RESEARCH PLAN

Domain "Informatics"

Sub-domain 01B1 "Informatics"

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Department of Physics

1. Research title

Convergence and integration of ICT computing paradigms and infrastructures for e-Science and SME.

2. Principal investigator

Andrea Bosin

3. Research team

Full professors	
Associated professors	
Assistant professors	Andrea Bosin
Post docs	
Ph. D. students	

4. ERC (European Research Council) research classification scheme

PE6_1	PE6_9	PE6_12

5. Key words

e-Science	Database	Cloud computing

6. National and international collaborations on this topic

Participation in the EU IMI Project "Molecular basis of the bacterial cell wall permeability" within the initiative "ND4BB Topic 2: Learning from success and failure & Getting Drugs into Bad Bugs".

Participation in the FutureGrid initiative founded by the US National Science Foundation, through the project "FG-157: Resource provisioning for e-Science environments" supported by a grant for the use of the FutureGrid computing infrastructure.

7. Abstract

The aim of this research is the study and the implementation of new models addressing the convergence and the integration of the different computing paradigms and infrastructures for the dynamic on-demand provisioning of the resources needed by e-Science environments and by SME requirements.

8. Framework and state-of-the-art

In the last years, the availability and models of use of networked computing resources are rapidly changing and see the coexistence of many disparate paradigms: high-performance computing, grid, and recently cloud. Unfortunately, none of these paradigms is recognized as the ultimate solution, and the convergence and integration of them all should be pursued.

9. Research description, milestones, and goals

Within the IMI project we will provide hosting facilities and informatics support for the very large tranche of Primary data generated within the computational and molecular modeling efforts in work packages WP5 and WP2. In addition we will work to implement consistent standards in handling of Primary data within the Public partners, through development and application of bespoke templates and process workflows. Project activities will span the years 2013-2017.

Within the FutureGrid initiative, we plan to work on the models for the convergence and the integration of the different computing paradigms and infrastructures, on their translation into working prototypes and on their application to significant case studies. In particular, one of the objectives is to endorse an open, flexible and modular workflow-based computing model, for example using the BPEL language. BPEL workflow design, nevertheless, is not straightforward even using the available graphical editors and, peeking at the business domain, the potential of the business process model and notation (BPMN) deserves some investigation given the capability of generating BPEL workflows directly from BPMN models. In addition, we plan to extend the existing prototype with the inclusion of new resource management systems and with the integration of both BPEL and non-BPEL workflow engines.

Another research activity targets cloud computing platforms for small and medium enterprises (SME). The specific objective is the development of platforms for cloud computing, and virtualization, flexible and adaptable to different domains (applications, operating systems, resources, storage, data access, etc.) with a minimal effort, effectively dealing with data security and privacy issues in an environment shared by many enterprises (even competing). The platforms will be developed making use of open-source solutions to avoid vendor lock-in. The choice of the most effective open-source solutions, and of the adopted standards, will constitute an important part of the research activity. Indeed, the fields of cloud computing and virtualization are rapidly evolving, and universally adopted standards are yet to come. Hence, the available solutions will be evaluated not only for their effectiveness, but also from the point of view of their appropriateness to the addressed potential market (enterprises, in particular local SME), and of the simplicity of migrating from one to another.