UNIVERSITY of CAGLIARI
Department of Physics

RESEARCH PLAN 2016-2018
of the
DEPARTMENT of PHYSICS

As approved on March 10, 2016

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

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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 whose 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 consists in:

- 7 full professors (PO)
- 18 associate professors (PA)
- 10 tenured assistant professors (RC-TI)
- 5 non-tenured assistant professors (RC-TD)

In addition, the DSF workforce includes approximately ten Post Docs, twenty Ph.D. students, and 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.

Specific information about research lines, networks of national and international collaborations, and 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 labelled 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 Institute 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).

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2. RESEARCH DOMAINS ACCORDING TO "EUROPEAN RESEARCH COUNCIL" (ERC)

The research activities here presented are labelled according to the general classification scheme of "European Research Council" (ERC).
Below is reported the ERC synopsis for the physical science

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

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
PE2_16 Metrology and measurement
PE3_13 Mesoscopic physics
PE2_17 Statistical physics (gases)
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

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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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PE9 Universe sciences:
astro-physics/chemistry/biology; solar system; stellar, galactic and extragalactic astronomy, planetary systems, cosmology; space science, instrumentation

PE9_6 Stars and stellar systems
PE9_10 High energy and particles astronomy – X-rays, cosmic rays, gamma rays, neutrinos
PE9_11 Relativistic astrophysics
PE9_15 Space Sciences

SH2 Institutions, values, beliefs and behaviour:
sociology, social anthropology, political science, law, communication, social studies of science and technology

SH2_14 History of science and technology

LS2 Genetics, Genomics, Bioinformatics and Systems Biology:
genetics, population genetics, molecular genetics, genomics, transcriptomics, proteomics, metabolomics, bioinformatics, computational biology, biostatistics, biological modelling and simulation, systems biology, genetic epidemiology

LS2_11 Computational biology

LS7 Diagnostic tools, therapies and public health:
aetiology, diagnosis and treatment of disease, public health, epidemiology, pharmacology, clinical medicine, regenerative medicine, medical ethics

LS7_2 Diagnostic tools (e.g. genetic, imaging)
LS7_11 Environment and health risks including radiation

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RESEARCH PLAN
Domain "Physics of fundamental interactions"
Sub-domain 02A1 "Experimental physics of fundamental interactions"

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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

Associated professors	Gianluca Usai, Alessandro De Falco
Post docs	Fiorella Fionda, Ester Casula, Elisa Incani
INFN researchers	Alberto Masoni (Direttore di Ricerca), Corrado Cicalò (Primo Ricercatore), Sabyasachi Siddhanta (tecnologo), Carlo Puggioni (grant position), Daniele Mura (grant position)

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 2016-2108 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 3μs 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.

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 $\rho(770)$, $\omega(780)$ e $\phi(1020)$ or heavier as the $J/\psi(3100)$, 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 2016-18 a new campaign of measurements of proton-Pb and Pb-Pb collisions will be performed. Within the approved experimental program, the research team will be involved in the following activities:

- Data taking proton-Pb, Pb-Pb
- Development of computing infrastructures based on the GRID technology for data analysis and data reconstruction.
- Study of low mass dimuon production in p-Pb and Pb-Pb collisions ($M<1.2$ GeV/c^2)
- Analysis of p-p collisions with high charge particle multiplicity
- Maintainance of the Muon Arm and Zero Degree Calorimeters (ZDC) detectors.

Besides those activities, the team is also involved in development of a new pixel vertex detector. The project was approved by the LHCC scientific committee during the 2012 fall. This detector will allow the production of charm and beauty mesons and baryons to be measured very precisely. The team will be involved in the following activities:

- Development and characterization of new pixel detectors

Responsibiities within the collaboration:

- Member of the experiment Editorial board (G. Usai)
- Conveener of the Physics Analysis Working group in charge for the analysis of low mass muon pairs (A. De Falco)

G. Usai is PI of the project “Study of monolithic pixel sensors for measurements in high energy nuclear collisions at the CERN LHC” (funded by Sardinia region).

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 the data analysis of the proton-nucleus data is still on-going. Two papers should be submitted in 2016-2017. At present a feasibility study is under way for a new muon spectrometer devoted to the investigation of chiral symmetry restoration and the first order transition of the hadronic matter phase diagram. A new PRIN project has been submitted, as a continuation of the previous lead by G. Usai (2011-13). The proposal is also under discussion with the italian heavy ion community within the INFN “What Next” initiative.

1. Research title

Physics of quarks and leptons: Heavy Flavours at LHCb
Novel techniques for axion detection

UNIVERSITY of CAGLIARI
Department of Physics

2. Principal investigators
Biagio Saitta

3. Reasearch team

Full professors	Biagio Saitta
Associate professors	
Assistant professors	Rudolf Oldeman
Post-docs	
PhD students	Violetta Cogoni, Claudia Vacca

4. ERC (European Research Council) classification scheme

PE2_1	PE2_2	

5. Keywords

Flavour Physics	LHC	Axions

6. National and international collaborations
- W. Bonivento, S. Cadeddu, A. Cardini, and A. Lai, researchers from the local section of the Istituto Nazionale di Fisica Nucleare (INFN) and the post-doc M. Fontana, 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 detectors development (principal investigator A. Lai) : University and INFN Padova, Pisa, Ferrara, Napoli.

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 in the years 2011-2012 enriched and statistically enlarged in a significant manner with new data acquired at the highest energy in the centre of mass ever reached at an accelerator. In particular it will address charm physics and rare decays of both charmed and B-mesons. In addition the group will contribute to the foreseen upgrade of the LHCb experiment,
in particular of its muon detector, taking advantage of the recognised expertise of some of its members in the development of detectors and electronics.
The development of novel detectors using scintillating fibres within the INFN project “Axioma” it is also expected.

8. 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?

With the discovery of the Higgs boson, the picture described by the Standard Model of particle physics is complete. To date, with few notable exceptions (one of which is the phenomenon of *neutrino oscillations*), there is no evidence for processes that can not be explained within the Standard Model thus requiring the existence of what is called "*new physics*".
Besides the observation, following direct production, of new particles whose existence is predicted by theories beyond the standard model – which is still possible at the higher energies available at present in proton-proton collisions at the accelerator LHC – evidence of *new physics* may be obtained indirectly through the analysis of decays of mesons and baryons containing heavy quarks and that are rare or forbidden in the Standard Model. Such decays, when mediated by new particles, would occur at a larger rate than predicted by the Standard Model.
The yield of particles containing heavy quarks (b and c) in the LHCb experiment is now orders of magnitude higher than achieved so far at any previous accelerator and with the increased statistics and with data at higher energies it will be possible to perform a wide range of measurements of unprecedented precision and to search for very rare decay modes and detect anomalies when compared to the Standard Model. A small discrepancy from Standard Model predictions has been observed in an observable in the angular distribution of the decay $B \to K^* \mu\mu$. Furthermore the ratio between the rate of this decay and the equivalent $B \to K^* e\, e$ seems to differ from unity suggesting a violation of lepton universality.

The axion is a particle postulated to resolve the problem of CP violation in Quantum ChromoDynamics. It could be one of the components of (cold) dark matter. However it has never been observed. It is proposed to develop, on a time scale of a few years, detectors featuring a novel technique that could be used for experiments aimed at the observation of axions.

9. Research description, milestones, and goals

LHCb – analyses. The new data sample recorded in 2015-2017 by LHCb will be used both to update and improve existing measurements and to start new analyses. In particular it is foreseen:

- To update the measurements of the ratio of branching fractions $B \to K^* \mu\mu$ to $B \to K^* e\, e$.
- To update the measurement of the absolute branching fraction of the decay $\Lambda c \to p\, K\, \pi$ using the novel method developed for this purpose.
- To measure for the first time the branching fraction of the decay $B \to p\, \pi\, \pi\, \Sigma c(2520)$ and if some conditions on the polarization are satisfied, to measure the spin of the $\Sigma c(2520)$.
- To analyse the decay of the neutral D-meson into two muons and into two muons plus 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 modes.
- To improve the algorithms for muon identification.

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. 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.

UNIVERSITY of CAGLIARI
Department of Physics

RESEARCH PLAN
Domain "Physics of fundamental interactions"
Sub-domain 02A2 "Theoretical high-energy physics"

1. Research title

Black holes and the gravity/gauge theory correspondence

2. Principal investigators

MARIANO CADONI

3. Reasearch team

Full professors	
Associate professors	MARIANO CADONI
Assistant professors	
Post-docs	
PhD students	EDGARDO FRANZIN, MATTEO TUVERI, PARUL JAIN

4. ERC (European Research Council) classification scheme

PE2_1 Fundamental interactions and fields	PE2_11 Relativity		

5. Keywords

Buchi neri	Corrispondenza gravità/ teorie di gauge		

6. National and international collaborations

S. Mignemi, Dip. Matematica, Università di Cagliari; V. Cardoso IST, Lisbona; P. Olla CNR

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 correspondence4
3. Microscopic entropy of black holes and other extended objects
4. Entanglement entropy of black holes
5. Shear viscosity to entropy ratio in QFT with gravitational duals

8. 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.

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.

Holographic description of critical systems

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 such as the shear viscovity to entropy ratio) of the duality.

Domain wall/cosmology correspondence

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.

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).

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'Alesio

3. Research team

Associate 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 (Univ. Torino), A. Prokudin (Penn State Univ., USA), E. Leader (Imperial College, UK), I. Scimemi (Univ. Complutense, Madrid, Spain), C. Pisano (Univ. Pavia), M. Echevarria (NIKHEF, Amsterdam); experimental groups (PAX, COMPASS, HERMES, JLAB, STAR, PHENIX, BELLE, BABAR).

7. Abstract

- Extraction (update) of transverse momentum distributions (TMDs) from experimental data in SIDIS and e^+e^- processes, with Q^2 evolution and inclusion of kinematical corrections;

- Estimates of single spin asymmetries (SSAs) for Drell-Yan processes and for inclusive W boson production

- SSAs in $l\, p \rightarrow \pi\, X$ and role of quasi-real photon exchange

- Role of TMDs in SSAs for single-inclusive hadron and jet-hadron production in proton-proton collisions;

- Process dependence effects and non-universality of TMDs

8. Framework and state-of-the-art

The understanding of the 3-dimensional structure of the nucleon, both in momentum and in coordinate space, is the ultimate goal of many ongoing or planned experiments and the focus of theoretical activities worldwide. The experiments are mainly high-energy scatterings of point-like leptons off protons and neutrons or inelastic collisions between nucleons. The theoretical scheme in which these processes are studied is QCD, both in its perturbative and non-perturbative aspects. The cross sections for the above processes are written, according to a factorization theorem, as the convolution of elementary partonic interactions - known from perturbative calculations in the Standard Model of strong and electro-weak interactions - with Partonic Distribution and Fragmentation Functions (PDFs and FFs). These are unknown, but their evolution with the large scale Q^2 of the process can be computed in QCD. Independent information on the FFs can be obtained from other processes, like the annihilation of e^+ and e^- into pairs of hadrons.
For a long time, the PDFs and FFs were considered as collinear splitting processes, which corresponds to a 1-dimensional imaging of the nucleon as a simple set of collinear partons. Recently, it has become

more and more clear that the understanding of many experimental results - in particular those involving spin degrees of freedom - must take into account the transverse degrees of freedom, that is the intrinsic motion of quarks and gluons inside the nucleons. This opens the way to the study of the 3-dimensional (3D) structure of nucleons.
The complete 3D information on the partonic momentum distributions has been encoded in Transverse Momentum Dependent Partonic Distribution Functions (TMD-PDFs). In experimental observables, they are often combined with Transverse Momentum Dependent Fragmentation Functions (TMD-FFs). A full knowledge of the partonic distributions must also include their dependence on hadronic and partonic spin, related to subtle spin-orbit correlations of the strong force. At leading order in 1/Q there are eight TMD-PDFs and, for spinless final hadrons, 2 TMD-FFs.
In the last 10-15 years the first measurements of azimuthal asymmetries in SIDIS (lepton + nucleon --> lepton + hadron +X) processes by the HERMES, COMPASS and JLab Collaborations, together with the related theoretical analyses, have definitely revealed the role of the TMDs and allowed the first extraction of some of them. Recent results by the Belle and BaBar Collaborations in e+ e- --> h_1 h_2 X processes have shown the role of TMD-FFs. Important data are expected soon from the Drell-Yan processes at COMPASS and RHIC. Great expectations are linked to the planned future Electron Ion Collider in USA and the AFTER experiment at CERN.
The QCD properties of the TMDs, in particular their QCD evolution with Q^2, have been studied: very recently, even if current phenomenological analyses present some controversy and require further developments. We are now in an important time of transition from a first introductory phase, which has established the basic experimental evidence and the theoretical framework, to a new precision phase for the exploration of the nucleon 3D structure.

9. Research description, milestones, and goals

Among the 8 independent TMD at leading twist, besides the 3 surviving in the collinear limit, the most studied ones are the Sivers and the Boer-Mulders functions, which give, respectively, the number density 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.
Recent theoretical developments on the QCD evolution of TMDs will allow improving their extractions through data analysis of semi-inclusive deep inelastic scattering (SIDIS) and e^+e^- annihilation processes. A global fitting procedure will be developed with dedicated numerical codes leading to new and update extractions of the Sivers and the Collins functions. [12-15 months]
Strongly related to this task, we will also compute theoretical estimates of SSAs for Drell-Yan processes and inclusive W boson production. These, when compared against the forthcoming data from COMPASS and RHIC experiments, would allow a clear, and still missing, test of the predicted change of sign of the Sivers function when moving from SIDIS to Drell-Yan processes. [6-8 months]

Still towards a better understanding of the properties of the TMDs, in particular of their non-perturbative part, an improved analysis of the q_T spectra in unpolarized Drell-Yan processes will be carried out. [6-9 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 the pion is produced with a large

transverse momentum. 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 deeper investigation. [6-9 months]
The study of azimuthal distributions of pions inside single-jet produced at large p_T in pp collisions will continue, with particular attention to the latest experimental results from RHIC, to have another source of information on the transversity distribution and test the universality of TMDs. [6-9 months]
We will also study the impact of quasi-real photon exchange in SSA for $l\, p \rightarrow \pi\, X$ (6 months), as well as potential sources of non-universality of TMDs by including initial and final state interactions in hadronic processes for the inclusive production of pions, jets, photons and bound states of the charm quark [12-15 months]

UNIVERSITY of CAGLIARI
Department of Physics

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

2. Principal investigators
Giuseppe D'Appollonio

3. Reasearch team

Full professors	
Associate professors	
Assistant professors	
Post-docs	
PhD students	

4. ERC (European Research Council) classification scheme

PE2_1	PE2_2	

5. Keywords

Superstrings and D-branes	Holographic duality	Higher spin fields

6. National and international collaborations
Paolo Di Vecchia, Nordita (Stoccolma) e Niels Bohr Institute (Copenhagen)
Rodolfo Russo, Queen Mary University London (London)
Gabriele Veneziano, Cern(Geneva) e College de France (Paris)

7. Abstract
The aim of our research project is to clarify how classical gravity effects, described in general relativity by the curvature of the spacetime, emerge from the string theory amplitudes and how string dynamics modifies classical gravity when the latter loses its validity (e.g. near a spacetime singularity such as a cosmological singularity) or whenever there is tension between the principles of quantum mechanics and the geometrical description of the spacetime (e.g. in the presence of an event horizon).

8. state-of-the-art
String theory is one of the most promising approaches to a quantum mechanical description of the gravitational interactions. The spectrum of the theory includes a massless spin-two particle, which can be identified with the graviton, together with an infinite number of massive particles of higher spin. String perturbation theory, an expansion in Riemann surfaces of increasing genus, defines a unitary scattering matrix. Constant advances in the field have significantly improved our understanding of what the essential features of a quantum theory of gravity should be. The most far-reaching discovery is perhaps the holographic duality between string theory in a curved spacetime and quantum field theory on the boundary of that spacetime.

9. Research description, milestones, and goals

Our research project aims at clarifying how string theory modifies the classical geometric description of the spacetime whenever this description becomes unreliable or leads to conclusions inconsistent with the principles of quantum mechanics. Our approach is based on the study of high energy processes in flat spacetime, in particular the collision of two ultra-relativistic closed strings or the collision of one closed string with a stack of D-branes. This provides a well-defined framework since the string S matrix ensures, at least in principle, the unitarity of the process. Even though the spacetime is initially flat, a curvature is induced dynamically by the high energy of the probes, that makes the exchange of gravitons the dominant interaction between the two strings or between the string and the D-branes.

At high energy it is necessary, in order to get consistent results, to resum the whole perturbative series. As shown by Amati, Ciafaloni e Veneziano in the case of string-string collisions, the resummation of the leading contributions in energy leads to an eikonal operator form for the S matrix. When the curvature radius of the spacetime is smaller than the string length, the eikonal operator provides a reliable description of the dynamics for every value of the impact parameter. In the opposite case, the eikonal operator captures only the limit of large impact parameter. The study of collisions leading to the formation of a black hole thus remains an open and challenging problem, since it is necessary to extract and resum a whole series of terms subleading in energy from the string amplitudes.

In the last few years my research activity was focused on the string-brane system. This system is an excellent framework to study the emergence of an effective geometry in string theory since the D-branes possess both a microscopic description (valid at weak coupling) in terms of open strings and a geometric description (valid at strong coupling) in terms of a class of curved backgrounds called extremal black branes. We showed that it is possible to reconstruct the metric from the string amplitudes at the leading and subleading order and we also analysed in detail the first process that signals a deviation from classical gravity, the excitation of the massive string modes caused by the tidal forces.

The next steps in this research project are the study of the absorption of the closed string by the D-branes [18 months] and the analysis of the effects of the tidal forces at the subleading order [18 months]. Concerning the first point, we plan to identify at the quantum and semiclassical level the open string state created on the branes, at tree level first and then taking into account the fragmentation induced by the higher terms of the perturbative series. Relying on this result we should be able to construct a unitary S matrix that in a narrow resonance approximation can simultaneously account for the elastic scattering, the tidal excitations and the absorption process. We would also like to investigate whether the excited D-brane system could provide a microscopic description of the near-extremal black branes. Concerning the second point, we plan to clarify whether the agreement between the string amplitudes and the background metric persists or not at the subleading order also for the tidal excitations and to devise methods to calculate the amplitudes at small impact parameter.

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title

Astroparticle Physics: Dark Matter and WIMP, signal directionality in DarkSide

2. Principal investigator

Alberto Devoto

3. Research team

Full professors	
Associated professors	Alberto Devoto
Assistant professors	Qui, Quo, Qua, ...
Post docs	
Ph. D. students	Matteo Cadeddu, Mauro Caravati

4. ERC (European Reserach Council) research classification scheme

PE_2	PE_4	

5. Key words

Dark Matter	Directionality	

6. National and international collaborations on this topic

M. Lissia, M. Razeti, researchers at the local section of the Istituto Nazionale di Fisica Nucleare (INFN), operating under the framework agreement between the University of Cagliari and INFN, are integral part of the group. Researchers coming from more than 50 Institutions from 10 countries (Europe, Brazil, China, and the United States of America) are actively engaged in DarkSide.

7. Abstract

During the next three years DarkSide 50 (the detector currently in use) will continue collecting data and, in parallel will continue the data analysis. Over the same time frame we will work on the design and the construction of a new much larger detector: DarkSide 20K.

8. Framework and state-of-the-art

A wide range of astronomical evidence implies the existence of dark matter, but as yet the nature of this major component of the universe is completely unknown. The large majority of physicists believes that about 85% of the matter in the universe is of a kind which does not absorb or emit electromagnetic waves:: i.e. dark matter. Most physicists think that dark matter is made of weakly interacting massive particles (WIMP's) whose nature is still unknown. At the present time there are many experiments engaged in the search for such particles, using different techniques. DarkSide is one of the experiments aiming for the direct observation of WIMP's through their collisions with the nuclei contained in the detector. For this reason it is necessary of highly purified materials, free for any "background noise" such as that produced by low levels of radioactivity (neutron emissions). Since

WIMPS are very weakly interacting, it is necessary to have large detectors. The results provided so far by DarkSide 50 indicate that a larger detector –such as DarkSide 20k- may provide important contributions in the search for Dark Matter.

9. Research description, milestones, and goals

The goal of this project can be achieved only using extremely pure materials and high sensitivity detectors. In particular the material used in the construction of the detector and its sensitive part has to be free from any source of neutron emitters. During the data run of 2015, the results so far obtained by DarkSide 50 have shown success of the techniques developed by the collaboration in order to eliminate the isotope Ar39 from the gas.

In the initial phase the collaboration will design and build the detector infrastructure, and the special photomultipliers necessary for revealing the photons produced in the collisions between WIMO's and Ar nuclei.

Between 2016 and 2018 the collaboration, and in particular the Cagliari unit, will be involved in the plant necessary for the production of Argon with ultra low levls of Ar-39. A 300 m high distillation tower will be built in Sardinia and Argon distillation will begin in the first half of 2017.

The efficiency and efficacy of the distillation process will be studied in collaboration with the Mechanical, Chemical and Materials engineering department of the University of Cagliari. The first results of the quality of the Argon will be available in early 2018.

The local group will also study from the theoretical point of view methods for detecting the directionality of WIMPS.

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
Nanomaterials for photonics and sustainable energy

2. Principal investigators
G.Bongiovanni, A.Mura, F.Quochi, M.Saba

3. Reasearch team

Full professors	*G. Bongiovanni*
Associate professors	*A. Mura, F. Quochi, M. Saba*
Assistant professors	
Post-docs	*D. Marongiu*
PhD students	*X. Chang, V. Sarritzu, N. Sestu*

4. ERC (European Research Council) classification scheme

PE3_12	PE4_3	PE5_4

5. Keywords

Nanomaterials	Photonics	Sustainable energy

6. National and international collaborations
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
We develop novel materials for sustainable energy and advanced photonics. Research activities will concern the design and photophysics of following materials: (i) hybrid metal-organic halide perovskites for advanced solar cells, LEDs and lasers; (ii) all-organic nanophotonic lasers and surface-plasmon nanolasers; (iii) lanthanide complexes for efficient NIR light emission and of porous metal-organic frameworks with luminescent building blocks for optical sensing of small molecules.

8. state-of-the-art
Nanomaterials 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 nanomaterials for low-cost solar energy conversion, novel light sources, chemical sensing and optical imaging.

9. Research description, milestones, and goals

Hybrid halide perovskites are a novel crystalline semiconductors combining the advantages of organic materials, such as easy and potentially cheap manufacturing, and those possessed by inorganic compounds, i.e. robustness and an excellent, balanced ambipolar charge transport character. We plan on ultrafast spectroscopy techniques such as transient absorption and time-resolved photoluminescence, employing laser pulses with different durations and repetition rates, to investigate the optoelectronic phenomena in perovskites. The scientific outcome will be the knowledge of materials parameters that control the lifetime in the excited state and unwanted recombination channels with the aim to find strategies to increase light emission and photoconversion efficiencies.

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.

Advanced organic-inorganic hybrid materials such as highly porous metal-organic frameworks (MOFs) will also be designed and photophysically investigated by means of transient photoluminescence and excited-state absorption spectroscopy with the aim to develop new materials for chemical sensing. Luminescent organic linkers such as anilato derivatives and/or NIR emitting lanthanide ions such as Er(III) and Yb(III) will be used to probe the adsorption of small molecules such as common air pollutants at the MOFs nanopores by optical sensing schemes.

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Novel fluorescent nanoarchitectures for photonic applications

2. Principal investigators
Carlo Maria Carbonaro, Riccardo Corpino, D. Chiriu

3. Reasearch team

Assistant professors	*Carlo Maria Carbonaro, Riccardo Corpino, Daniele Chiriu*

4. ERC (European Research Council) classification scheme

PE4_1	PE4_3	PE5_6

5. Keywords

Nanomaterials	Photonics	Optical Spectroscopy

6. National and international collaborations
M.F. Casula,C. Cannas, A. Salis, Dept. of Chemical and Geological Sciences, University of Cagliari; A.Corrias, G. Mountjoy, School of Physical Sciences, University of Kent; D. Carta, Fac. of Physical Sciences and Engineering, University of Southampton; A. Falqui, A. Casu, King Abdullah University of Science and Technology, M. Cannas, S. Agnello, Dept. of Physics, University of Palermo; S.Gerard, Y. Ouerdane, Laboratoire Hubert Curien, Univ. de Saint-Etienne; L. Malfatti, Faculty of Architecture, University of Sassari; A. Paleari, Dept of Materials Sciences, Univeristy of Milano-Bicocca.

7. Abstract
The research project aims to investigate novel fluorescent nanoarchitectures to engineer organic-inorganic hybrids for applications in photonics (white LED and nanolasers). The selected fluorescent compounds are Carbon-dots (CDs) whose emission properties can be tuned by quantum confinement and surface functionalization. To achieve photonic applications the fluorescent compounds will be embedded in suitable matrices, such ordered mesoporous silica.

8. state-of-the-art
Carbon dots (CDs) are a novel family of C-nanoparticles attracting academy interest because of their capability of yielding bright and tunable fluorescence. In addition, these compounds possess water solubility, low toxicity, photo-stability, and a versatile photochemistry, envisaging applications in bio-imaging optoelectronics, photocatalysis and solar energy harvesting.

Chemical and physical procedures to produce CDs are in general facile, green, and low-cost, the C-source ranging from charcoal to candle soot, orange juice, or potatoes. However, the structure, composition and therefore optical properties of CDs are rather synthesis-dependent. In addition, beside carbon, CDs usually contain large amounts of oxygen (20-40%), especially at the surface, and nitrogen is often introduced as dopant up to rather large concentrations to increase emission performances. Up to now, most studies on CDs have addressed their properties in liquid phase, in

particular water. Only in recent times, an increasing effort is being devoted to develop CD-based solid materials, in view of the potential solid-state applications of their light emission.

9. Research description, milestones, and goals

The project aims to study C-dots-based nanocomposites for solid-state lighting and lasing applications. Following the lead of green chemistry and the priorities of H2020, the use of C-dots would allow reducing the use of poisoning heavy metals, (Cd, Sb, Pb, etc.) or rare earths elements (La, Er, Ga, etc.), largely applied for photonics solutions. Nowadays the fluorescent quantum yields of C-dots in the blue/green range is almost competitive to those of CdSe/ZnS, however, the emission efficiency of C-dots in the red/near-IR range should be improved. The first target of the project is therefore to exceed this deficit and the design of a C-dots-loaded matrix showing an efficient emission of white light. C-dots will be designed using both chemical and physical processing, and the emission will be tuned to achieve a variety of colours and compose the white light. The emission will be also maximized through surface functionalization or by means of coupling with plasmonic metal nanoparticles. One-pot synthesis, post-functionalization of a porous matrix and ship-in-a-bottle approaches, through in situ C-dots synthesis, will be used to prepare highly-loaded matrix made of hybrid organic-inorganic or polymeric materials. The overall properties of the materials, in terms of colour rendering and temperature, thermal and chemical stability will be tuned using the wide flexibility offered by the sol-gel approach. The chosen host matrix is ordered mesoporous silica because its huge specific surface area allows hosting large concentrations of fluorescent CDs. The analysis of the interaction of CDs with the matrix, in terms of physical and chemical confinement of emitting compounds, is a strategic issue to fill the current knowledge gap about CDs in embedded systems. The research activity is planned for a period of three years and is divided in three work-packages (WPs). WP1: synthesis, functionalization and characterization of silica based ordered mesoporous materials (OMM) with ordered and controlled porosity. WP2: synthesis and characterization of CDs with different chemical and physical procedures and starting from different C-sources. WP3: embedding of CDs in silica matrix and characterization of their spectroscopic features. The proposed research is multidisciplinary and will be carried out in close collaboration with the Department of Chemistry and Geology and the other academic collaborations of the research team. The project is under evaluation within the call for research base project of MIUR (year 2015).

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	

4. ERC (European Reserach Council) research classification scheme

PE3_1	PE3_8	PE3_10

5. Key words

Magnetism	Nanomaterials	Molecular Materials

6. National and international collaborations on this topic

ISM-CNR, Unity of Montelibretti (RM)
Dipartimento di Scienze Chimiche e Geologiche, Università di Cagliari

7. Abstract

The objective of this project proposal is the investigation of the magnetic properties of low dimensional systems, such as magnetic nanomaterials and multifunctional molecular materials.

8. Framework and state-of-the-art

The determination of the dependence of the magnetic properties on the size and shape of the nanoparticles and on the structure of the molecules is the objective of this project. Relevant magnetic nanoparticles are formed by an oxide or they are nanocomposites of two different oxides. Multifunctional molecular nanomaterials are constituted by an anionic complex of transition metals (magnetic component) and from an organic molecule (component electrical conductor).

9. Research description, milestones, and goals

The magnetic properties of nanomaterials and molecular materials will be studied using the magnetic SQUID magnetometer (Quantum Design MPMS XL5, USA) of the research group. The magnetometer measures the dc (direct current) magnetization with applied magnetic fields up to 5 T, in a temperature range from 400 K to 1.9 K, with a sensitivity to the magnetic moment of 10-6 erg/G. This allows you to determine if the material is in a disordered state (diamagnetic or paramagnetic) or ordered (antiferromagnetic or ferromagnetic). By measuring the magnetization as a function of temperature, it may determine the magnetic transition temperatures (Curie or Neel). By measuring instead the magnetization as a function of the field, you can determine the hysteresis loop and the characteristic parameters of a ferromagnet (coercive field, residual magnetization and saturation), fundamental for the purposes of possible applications. The Fe-containing materials can also be studied by Mössbauer spetroscopy of Fe-57. The group works with three Mössbauer spectrometers for low-temperature measurements from 300 K to 4 K (with a cryostat at liquid helium) and high 300 K to 1000 K (with a vacuum chamber). This spectroscopy shows the state of magnetic order; it also also allows you to measure the volume fraction ordered, if other than 100%; this is not possible with the SQUID magnetometer.

Will be studied also particularly important aspects such as:

- The possibility of interplay between the conduction electrons delocalized and the localized magnetic moments;
- The effect of a magnetic field on the transport properties of a ferromagnetic conductor;
- The possible coexistence of ferromagnetism or antiferromagnetism and superconductivity in molecular materials.

UNIVERSITY of CAGLIARI
Department of Physics

Preventivo 2016-2018 Congiu -Geddo Lehmann Inglese

1. Research title
Ferroic perovskites: structure-properties relationships in bulk, thin films and nanoparticles

2. Principal investigators
Geddo Lehmann Alessandra and Congiu Francesco,

3. Reasearch team

Full professors	
Associate professors	
Assistant professors	*2*
Post-docs	
PhD students	

4. ERC (European Research Council) classification scheme

PE3_8	PE5-6	PE3-10

5. Keywords

Perovskites	Ferroicity	Phase transitions

6. National and international collaborations
CNR-SPIN-Naples
Dipartimento di Ingegneria Industriale, Università di Salerno
CNR-Rome

7. Abstract
Ferroic and multiferroic perovskites present many interesting properties, such as (anti)ferroelectricity, (anti)ferromagnetism, magnetoelectricity, superconductivity. As such, they are widely studied for applications as functional materials. Our research team in engaged in the study of some classes of functional perovskites, to the aim of clarifying the relationships between their crystal structure and microstructure and ferroic properties.

8. State-of-the-art
Although perovskites have been known and studied since 1839, year of the classification of $CaTiO_3$ as a mineral, new properties are continuously discovered in materials belonging to this structural type. Recent examples are Mn oxides showing colossal magnetoresistance or mixed organic/inorganic halides which have been proved to have outstanding photovoltaic response. Therefore their study still remains a highly competitive research field in condensed matter physics. Hot topics in perovskites are multiferroicity, search for green, lead-free piezoelectrics/ferroelectrics and relaxors, emerging phenomena at interfaces, either at heterointerfaces between different compounds or at ferroic domain

boundaries, the role of spontaneous polarization and ferroelectric domain walls in the photovoltaic response of both oxides and halides. Our research aims at enlightening several aspects of the previous topics, some of which have been the object of intensive research within the Italian project PRIN OXIDE just concluded.

9. Research description, milestones, and goals

1)Properties of interfaces in perovskites (2016).

1a) We shall study the magnetic and charge transport properties of colossal magnetoresistive manganites containing natural interfaces in the form of ferroelastic domain walls. To this aim, epitaxial films with stripe structural domains will be analyzed, the twin structure of which scales with thickness following the Kittel's law. We shall conclude the experimental work already performed on La-Sr-Mn-O films, and shall discuss the correlation between the magnetic response and the ferroelastic domain structure.

1b) We shall conclude the study of the magnetic response of epitaxial films of Pr-Ca-Mn-O CMR manganite on $NdGaO_3$ in different crystallographic orientations, by comparing SQUID magnetometry and MOKE results. The role of proximity effect in the magnetic anisotropy and exchange bias will be discussed.

2) Phase transitions in nanostructured Mn perovskites (2016-2017).

2a) The study on the use of the magnetocaloric effect as a tool for studying of the magnetic and magnetostructural/magnetoelastic transitions in CMR perovskites will be concluded. In particular, results obtained on the system Pr-Ca-Mn-O will be published.

2b) A comparison of the phase transitions between bulk and nanoparticles of the multiferroic system Ho-Ca-Mn-O will be carried out. In particular, the charge ordering destabilization in nanoparticles will be discussed.

3) Ferroelectric perovskites for photovoltaics and photocatalysis: synthesis, structural and dielectric characterization (2016-2018).

In the field of ferroic ferroelectrics, we plan to carry out the synthesis and the characterization of perovskites with potential applications in solar energy conversion, and to study the role of polarization and/or ferroic domains in their photoresponse. This is a topic known since about thirty years, that however aroused a new interest after the discovering of the huge photovoltaic response of hybrid organic/inorganic halides with incipient ferroelectricity. Materials will be chosen among three dimensional or layered perovskites on the base of the value of their absorption edge. For oxides, ceramics samples will be prepared by solid state reaction and successive sintering of highly dense pellets. Structural characterization will be performed by powder X-ray diffraction. Dielectric characterization will be carried out by a Radiant Tester through the collection of P(E) loops and by measuring the dielectric constant as a function of frequency and temperature. Selected samples will be thereafter tested for their photoresponse.

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title

Porous silicon for technological applications

2. Principal investigators

Guido MULA

3. Reasearch team

Full professors	
Associate professors	
Assistant professors	*Guido Mula*
Post-docs	
PhD students	*Mariavitalia Tiddia*

4. ERC (European Research Council) classification scheme

PE5_6	PE5_8	PE4_1

5. Keywords

Porous silicon	Hybrids organic-inorganic	Rare earths

6. National and international collaborations

- A. Falqui, (BESE), KAUST, Jeddah, Kingdom of Saudi Arabia
- A. Pezzella, Dip. di Scienze Chimiche, Univ. Federico II di Napoli, Napoli
- M. Mascia, S. Palmas, A. Vacca, DIMCM, Univ. Cagliari
- N. Gambacorti, T. Printemps, P. Bleuet, CEA, LETI, MINATEC Campus, Grenoble, France
- F. d'Acapito, CNR-IOM-OGG c/o LISA - ESRF, Grenoble, Francia

7. Abstract

In the 2016-2018 years we will focus our activities on the organic-inorganic hybrids of polymers (e.g. polyaniline and melanins) and porous silicon. These structures will be mainly studied by optical, electrical, electrochemical and structural means. Lithography on nitrobenzene-functionalizes porous Si will also be approached. We will also continue the study of the electrochemical doping of porous Si with rare earths and metals for the improvement of the photoluminescence efficiency and study other material characteristics of the material, e.g. structural properties.

8. State-of-the-art

Porous Si (PSi) is a very versatile material used in a very wide range of applications. Recently, its application for hybrids devices has been drawing increasing attention from the scientific community. Given the peculiar structure of the inner PSi pores structure, it is a major scientific challenge to understand the impregnation mechanisms and the hybrid interface formation processes. The dendritic PSi structure implies a strong

dependence of the internal electric fields on the exact location within the structure and that it is then difficult to accurately control the ability of the impregnating solutions to fully penetrate the pores.
The complex pores' structure is also at the origin of the insufficient information to explain the lack of efficient luminescence from Er-doped PSi. The improvement of the PSi:Er system requires a better knowledge of the mechanisms underlying the Er-containing solution penetration within the porous structure and can only be achieved through improved up-to-date characterization of the samples.

9. Research description, milestones, and goals

In the 2016-2018 years we plan to study hybrid bulk heterojunctions made by the insertion of polymers into the PSi matrix and to improve the characterization of PSi:Er systems. In details:

1) *Research on hybrid junctions*. The junctions will be fabricated starting from pristine or lightly modified PSi samples and polymers as melanins and polyaniline. The characterization of the samples will be performed by several means: optical reflectivity, Scanning Electron Microscopy, Photoconductivity, I-V scans, electrochemical impedance spectroscopy. The research activity will also focus on the effect of chemical and electrochemical modification of the inner surface of the PSi pores to improve the stability of the organic-inorganic interface. In fact, the short lifetime of the devices is incongruent with the lifetime of the junction components and is related to the interface instability due to chemical and structural reasons. The modification of the pores surface and/or the polymers fabrication process and composition will be made with the goal of understanding and optimizing both the efficiency and the stability of the hybrids.

2) *Research on doped PSi*. The fabrication process of PSi:Er for strong photoluminescence needs a precise knowledge of the effect of each fabrication step on the final results. The principal focus of our research will be on the characterization of the samples as a function of the different process parameters, for which we plan to use, in addition to other techniques, 3D electron tomography to achieve detailed structural information at the nanoscale. We also plan to obtain detailed PL mapping of the samples (we plan to reach a spatial resolution in the order of a few hundreds of nm) both on the top surface and on the cross section to identify a route towards the optimization of the PSi:Er structure from the PL point of view. To reach this goal, we will modify the electrochemical Er impregnation, the thermal treatment and other parameters in each of the delicate steps of the fabrication procedure.

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title

"Optical and structural characterization of CRM free materials for optoelectronics applications."

2. Principal investigator

Pier Carlo Ricci

3. Research team

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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

- A. Rizzi - Physics Department Georg-August University of Göttingen
- S. Cuesta-Lopez, Advanced Materials - University of Burgos
- J. A. De Toro Sanchez – UCLM
- F. Beolchini - Università Politecnica delle Marche – UNIVPM
- S. Fuendling, A. Waag Technische Universität Braunschweig;
- Maria Luisa Grilli (ENEA).

7. Abstract

The Research activity will be focalized on development of Critical Raw Materials (CRM) free devices for electronic and optoelectronic and related to the topic of the EIP commitment RESET. The theme of the recycle will be analyzed and in particular, the possibility to utilized the CRM waste for new devices will be explored. The optical and structural properties will be characterized mainly by Raman spectroscopy, Steady time and Time resolved luminescence in different temperature conditions.

8. Framework and state-of-the-art

Raw materials are fundamental in most technological applications, however some of them are being recently defined by the EU commission as "critical" due to the high risk of supply shortage expected in the next 10 years and for their importance in the European Industry.
Different devices utilize nowadays compounds with CRMs as key elements, from lighting devices, (LED, OLED, CFL: Rare earths, like Ce, Y, Eu and Tb, In as CRMs), to optoelectronics, such as transparent conductive layers (In as CRM), permanent magnetic materials (in SmCo, NdFeB). Research is needed to improve the fundamental understanding of the development of new material solutions with a reduced or completely eliminated critical content, while maintaining or enhancing the performance of the materials, components and products.

The design of the alternatives compounds, the control of growth process coupled with accurate characterization are mandatory for further development of new CRM free devices.

9. Research description, milestones, and goals

The framework of the proposed research activity is within the research interests of the EIP commitment RESET: Raw Elements Substitution in Electronic and optoelectronic Technologies.
The research activities is divided on three principal field,

- Hybrid Organic/Metal oxides system
- Nanocomposites for magnetically-induced luminescence
- Optical and structural properties of field effect organic biosensor.
- Alternative phosphors for GaN based 3D-LEDs.

In the first project, in collaboration with University of Ghent, FBK Trento and the department of Chemistry of the university of Cagliari, the structural and optical properties of different Metal oxides/organic hybrds systems will be explored. The realization of a hybrid system can provide significant benefits to the optical response of oxide material. The new features of the phosphor was explained by the presence of two effects, an efficient organic to lanthanide energy transfer and the decreasing of quenching effect due to surface defects. In this context, it is important to realize the synthesis process, occurred at high temperature, preventing the saturation of defects with OH species. The realization of multishell system will be also explored.

Magnetically induced Luminescence (MIL) is a forefront research field that requires the cross knowledge of different specific fields of Materials Science, from magnetism to nanosized effect, from structural characterization to luminescence. Only few months ago it was proved in few high Impact Factor publications that the MIL effect can be relatively easily accessible by using magnetic materials embedded in flexible laminate structures coupled with piezophotonic materials.

The research in this topic is at the very beginning and new characterizations and, more in general, deeper studies are mandatory. On these basis the prompt collaboration in an international network can be strategic both from the base research point of view and for future innovative applications. This topic will be firstly developed in collaboration with the the Applied Nanomagnetism Group of the
Universitad de Castilla - La Mancha (Spain).

The theme of new lighting systems and in particular LED technology will be fundamental in the next years. However,a drastic reduction of production cost and energy consumption is needed. As a result, the research in this field has large interest from a scientific point of view, with focus on the development of new hybrid organic/inorganic phosphor and cost efficient 3D-InGaN structures and further strategies especially for immediate applications in market products. In order to provide a “defined standard”, conventional broad area LED chips and 3D-structured LED chips of the same kind will be provided by TU Braunschweig (Germany). The LED chips will be coated with alternative phosphor materials, developed by University of Cagliari.

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Development of spectroscopic techniques for non-destructive investigations of archeological artifacts

2. Principal investigators
Marcello Salis

3. Reasearch team

Assistant professors	*Daniele Chiriu*

4. ERC (European Research Council) classification scheme

PE4-2	

5. Keywords

Optical spectroscopy	Luminescence	

6. National and international collaborations
Nadali Davide (Università degli Studi di Roma "La Sapienza"); Polcaro Andrea (Università degli studi di Perugia)

7. Abstract
The research project is devoted to the development of an handheld instrumentation based on the combination of micro-Raman spectroscopy, XRF and OSL for the investigation in situ of archeological artifacts that cannot be moved in a laboratory. The Raman and XRF techniques provide useful information for structural and compositional characterization of artifacts and hence for the identification of their geographical region of origin. The OSL technique allows for the luminescence dating of examined samples thus providing information about their historical period.

8. state-of-the-art
Specific analysis of ancient artefacts by non-destructive and non-invasive means is a topical issue in the field of Cultural Heritage. In this connection, numerous papers could be cited for the use of Raman spectroscopy applied in Cultural Heritage. The role of Raman spectroscopy in the identification of pigments used in ancient painted walls and decorative potteries is already ascertained. In addition to Raman spectroscopy, XRF technique provides one of the simplest, non-destructive most accurate and most economic analytical methods for the determination of the chemical composition of many types of materials. The physical limit related to the investigation of low atomic number elements could be easily resolved by using the Raman technique, complementary to the XRF technology. Luminescent materials are suitable for retrospective dosimetry using no destructive Optically Stimulated Luminescence (OSL) analysis (such as clays, quartz, feldspar, aluminium oxide etc.).
Luminescence dating is based on a combination of retrospective dosimetry and environmental dosimetry.

9. Research description.
The research project will be dedicated to the realization of experimental setups for measurements on ancient artifacts indicated by the collaborators of Rome and Perugia.

1st year:
The experimental setup will assembly a portable IR Raman spectrometer with a XRF spectrometer, in micro and macro configuration, with the possibility to generate compositional mapping of the analyzed samples. Collected data will be processed and a first interpretation of materials and conservation status will be shared with the collaborators of Rome and Perugia for an accurate archaeological analysis.
2nd year:
An additional experimental setup for OSL analysis will be integrated in the above system with the purpose to date the studied samples. The results will be generated by a combination of collected OSL data, a model of trapping processes and kinetic recombination, and NORM (Naturally Occurred Radiative Materials) analysis of the geographical context related to the samples.
3rd year:
The validation of the above techniques will be assured by the comparison of the experimental results and literature information about test samples. All the scientific investigation will be realized with the strict synergy among the involved collaborations.

UNIVERSITY of CAGLIARI
Department of Physics

RESEARCH PLAN nel
Domain "Condensed matter physics"
Sub-domain 02B2 "Theoretical condensed matter physics"

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UNIVERSITY of CAGLIARI
Department of Physics

1. Research title

Investigation of hidden parameters in unconventional superconductors.

2. Principal investigators

Fabio Bernardini

3. Reasearch team

Full professors	
Associate professors	*Fabio Bernardini*
Assistant professors	
Post-docs	
PhD students	

4. ERC (European Research Council) classification scheme

PE3_6 Macroscopic quantum phenomena: superconductivity, superfluidity, etc	PE3_4 Electronic properties of materials, surfaces, interfaces, nanostructures, etc.	PE5_2 Solid state materials

5. Keywords

UNCONVENTIONAL SUPERCONDUCTIVITY	IRON BASED SUPERCONDUCTORS	INTERPLAY BETWEEN SUPERCONDUCTIVITY AND MAGNETISM

6. National and international collaborations

Brian M. Andersen, Niels Bohr Institute, University of Copenhagen.
A. Cano, Institut de Chimie de la Matière Condensée de Bordeaux CNRS , Francia
Prof. N. Saini, Dipartimento di Fisica, Università di Roma "La Sapienza"
Dr. S. Sanna, Dipartimento di Fisica, Università di Pavia.
A. Martinelli, SPIN-CNR, Genova.

7. Abstract

I will study the origin of unconventional superconductivity in the iron-based superconductors. Special attention will be devoted to the so-called hidden parameters dominating the superconducting behavior. Density functional theory (DFT) calculation will be used to compute the U (Coulomb repulsion) and t (hopping intergral) parameters used in the modeling of the magnetic interactions.

8. state of the art

Superconductivity intrigued scientists ever since its discovery in mercury in 1911.
During the past few decades several new classes of unconventional superconductors have been discovered, such as cuprates, Fe-pnictides/chalcogenides as well as some heavy fermion and actinide materials.

Nowaday, even after large research efforts, not all classes of superconducting materials are fully understood. There are now accumulating evidences that competition/interplay between spin, charge and orbital ordering is often at play
in unconventional superconductors suggesting that they share a common underlying physics. Fluctuations of a suppressed order are often invoked as pairing glue in the superconducting mechanism. A variation of this conceptual framework is to involve quantum fluctuations around a Quantum Critical Point where two
competing orders are suppressed at zero temperature.

9. Research description, milestones, and goals

The aim of my activity is to unveil the intimate physical parameters (hidden parameters) that govern unconventional superconductivity in the iron-based superconductors (IBS). In particular the main purpose is to understand and quantify which degree of freedom among spin, charge or structure are determinant to destroy/induce the superconductivity in these materials.
This final and ambitious aim, can be approached by achieving the following intermediate targets:
1) To identify the regions of the phase diagram where magnetic fluctuations dominate.
2) To search for charge ordering signatures and explore its dynamics.
3) To identify the role of local distortions (orbital or lattice driven) in the superconducting pairing.
The trends of these three ingredients shall be probed across the phase diagram of carefully selected IBS materials. I will concentrate my attention on the 1111 family (e.g. LaFeAsO). In this material superconductivity and magnetism can be tuned my the substitution of Fe with Mn and La with a rare-earth.
The hidden parameters that govern unconventional superconductivity can be unveiled by identifying the coexistence regions of the different ordered phases and the behaviour of their order parameters and transition temperatures
(Néel temperatures, critical temperatures Tc, charge-ordering and local
structural transitions, etc). Particular attention will be devoted to the study of correlation between spin fluctuations and $T_{C.}$
DFT calculations will provide the electronic band structure for the systems under investigation following a well-established theoretical-experimental collaboration with the Dipartimento di Fisica dell'Universita of Pavia and the laboratory SPIN-CNR of Genova. Particular attention will be devoted to the effect of chemical pressure on the ratio U/t between Coulomb repulsion and hopping integral. This will allow us to understand if the suppression of magnetic order is due to a reduction of the electronic correlation. The U and t will be important in the real-space description of the magnetic interaction in the presence of Mn impurity according to the RKKY model.

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title

Electronic and optical properties of materials (from organic and biological molecules to inorganic crystals)

2. Principal investigators

Prof. Giancarlo Cappellini

3. Reasearch team

Full professors	
Associate professors	Giancarlo Cappellini
Assistant professors	Andrea Bosin
Post-docs	Elena Molteni
PhD students	Roberto Cardia

4. ERC (European Research Council) classification scheme

PE3_5	PE3_7	PE2_8

5. Keywords

Solid State Physics	Theoretical Spectroscopy	Organic and Biological Molecules

6. National and international collaborations

Dr.ssa Maurizia Palummo, Dipartimento di Fisica, II Università di Roma ''Tor Vergata''
Prof. Giovanni Onida, Dipartimento di Fisica, Università di Milano
Dr. J. Furthmueller, IFTO-FSU Jena ,Germany
Prof. Gian-Marco Rignanese, NAPS, Université Catholique de Louvain, Belgium
Dr. D. Chiriu, Dipartimento di Fisica, UniCa

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) Organic and biological molecules.
These issues will be treated within computational simulation techniques.

8. State of the art

Spectroscopic techniques play a fundamental role in the study of the electronic and optical properties of solids, molecules and atoms.
The introduction of computational codes, named ab-initio ones, for the calculation of

the electronic properties of localized and extended systems have improved the capability to understand the electronic and optical experimental spectra of different systems. In fact 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 the main goal of the present research plan.

9. Research description, milestones, and goals

The paramete-free computational codes devoted to the calculation of the spectroscopic properties of materials can be of different kind: DFT-LDA and DFT-GW schemes for the ground and excited electronic states,TD-DFT or BSE ones for the optical spectra.
More info about techniques, their origin, the comparison with experimental results could be found at the web site of ETSF (European Theoretical Spectroscopy Facility) network http://www.etsf.eu.
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.
Ionic crystals with the fluorite structure show large band-gap and high transparency in a wide-frequency range. After we have studied CdF_2 and BaF_2 we plan to extend our interest to different systems (e.g. MgF_2 ore SrF_2). Moreover we plan to make comparisons within different computational schemes on the electronic ground and excited states/optical properties of bulk fluorite sytems to test which shows the best performances in term of saving of computational resources. These actions aim to seek an efficient method to tackle more complicated systems (e.g. surfaces, bulk-defects, surface-defects, interfaces) which play an important role in fluorides based applications/materials.

B)Electronic and optical properties of organic and biological molecules

The use of the above mentioned computational techniques had a strategic importance in the last years for the calculation of the electronic and optical properties of molecules of interest in different fields: from astrochemistry and astrobiology to materials science and cultural heritage.
Between the molecular species interesting in the above fields the molecules of carbonaceous basis are of fundamental importance; in particular the polycyclic aromatic hydrocarbons (PAHs) and their derivaties should be one of the most abundant families in space. These molecules are of importance also for optoelectronic applications when considered in their solid phase. Moreover we would like also to consider biomolecules as the nucleobases (e.g. thymine (DNA) and uracil (RNA)) for astrochemistry/biology interest and potential materials science applications.
For cultural heritage researches we would like also to consider within different techniques organic systems as cellulose and the benzoquinones.

UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Theory and simulations of nanomaterials

2. Principal investigator
Luciano Colombo

3. Reasearch team

Full professors	Luciano Colombo
Associate professors	
Assistant professors	Claudio Melis
Post-docs	• 1-2 post-docs are expected to be hired in this 3-year period
PhD students	• Riccardo Dettori • 1-2 PhDs are expected to be hired in this 3-year period

4. ERC (European Research Council) classification scheme

PE3_3	PE3_7	PE5_10

5. Keywords

Atomistic simulations	Nanomaterials	Thermal transport

6. National and international collaborations
- Institut de Ciència de Materials de Barcelona((ICMAB-CSIC), Spain
- Universitad Autonoma de Barcelona, Spain
- Catalan Insitute for Nanoscience and Nanotechnology (CIN2), Barcelona, Spain
- University of Califoria at Davis (USA)
- Institute for Polymer Physics, MPI-Mainz, Germany
- Ècole Polytechnique, Palaiseau, France
- Institut d'Electronique, de Microélectronique et de Nanotechnologie (IEMN-CNRS), Lille, France
- Norwegian University of Science and Technology, Trondheim, Norway
- Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy
- Università di Milano-Bicocca, Italy
- Istituto Officina dei Materiali (CNR), Cagliari, Italy
- Istituto Nazionale di Ricerca Metrologica (INRIM), Torino, Italy

7. Abstract
We will focus on the theory & simulation of novel nanomaterials for advanced applications, including: energy harvesting & production (i.e. thermoelectric and photovoltaic conversion), manipulation of thermal transport in nanoelectronics, elasticity of nanocomposites, and systems for metrological research.

We will as well develop, implement, and apply new computational methods for large-scale atomistic simulations.

8. State-of-the-art

Modern simulations enable the quantitative prediction and rational screening of materials properties, as well as the design of new devices based on them.

A combination of elements has detemined this success: theoretical research has transformed abstract ideas and equations into algorithms; applied research has turned these algorithms into powerful and flexible codes; codes benefit of the ever increasing computational power; the extensive cross validation of the resulting computational tools against experiments provides us the confidence necessary to undertake applications of ever increasing complexity.

The level of maturity and flexibility of modern simulations makes them applicable to a range of problems unthinkable up until recently: from materials, to chemistry, engineering, and biology to name a few.

By computer experiments performed with state-of-the-art simulation methodologies we will develop new fundamental knowledge -targeted to advanced applications- on nanomaterials.

9. Research description, milestones, and goals

- Heat transport in glassy materials
  Glassy materials (intermediate between liquid and solid) have paramount applications in technology. Notwithstanding, the temperature dependence of their thermal conductivity remains unexplained, especially at low temperature.
  By nonequilibrium molecular dynamics (NEMD) simulations and modified Boltzmann transport equation calculations we will investigate thermal conduction in realistic glass models over the full temperature range of fundamental and practical interest.
- Interface thermal transport
  Thermal transport properties of interfaces, namely Kapiza resistance (KR) and thermal rectification (TR), between unlike materials are still poorly understood.
  By NEMD we will investigate KR and TR performances for a number of prototypical interfaces (occurring in nanostructured semiconductor, as well as in polymer-semicondutor composites or polymer bundles) useful for thermoelectric conversion, heat evacuation or phononics.
- Thermal transport properties in 2D materials
  The above concepts, theoretical methods, and simulation tools will be applied to study thermal transport in 2D atomic sheets like, e.g., graphene, boron-nitride, MoS_2 in realistic structural conditions (i.e. including defects, grain boundaries, and borders) of current interest in nanotechnology.
- Multiscale modeling of elastic properties of Si surfaces
  By combining continuum elasticity with MD simulations and ab initio total energy calculations, we will investigate the elastic fields occurring at/nearby non-ideal (i.e. curved, defected, oxidized or loaded) Si surfaces relevant in nanocomposite technology or in metrological research.
- Thermal dissipation in complex fluids
  By developing new NEMD simulation methodologies we will investigate the heat dissipation phenomena in complex H-bonded liquids. In particular, we will focus on the fundamental

understanding of “pup&probe” experiments aimed at characterizing the relaxation dynamics of single laser-excited vibrational states.

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UNIVERSITY of CAGLIARI
Department of Physics

1. Research title

Unconventional ferroelectric and semiconducting oxides for electronic applications

2. Principal investigator

Vincenzo Fiorentini

3. Research team

Full professors	
Associate professors	*Vincenzo Fiorentini*
Assistant professors	
Post-docs	
PhD students	
Laurea students	*Andrea Urru*

4. ERC (European Research Council) classification scheme

PE3_5 Electronic structure	PE3_4 Semiconductors	PE5_8 New materials

5. Keywords

Ab initio theory	Ferroelectricity	Wide-gap semiconductors	Alloys

6. National and international collaborations

- CNR-SPIN Genova: oxide interfaces
- CNR-ISM Roma: oxides for electronics
- Uni Parma: oxides for electronics
- Luxembourg institute of Science and Technology: ferroelectrics

7. Abstract

For the foreseable future, we will continue developing and applying new ab initio methods to two large families of materials: a) systems with magnetic, dipolar, orbital, charge, etc. order; b) oxide wide-gap semiconductors. Our goal applications are, respectively, metallic ferroelectrics and ternary (Ga/Al/In)O alloys, with collaborations, including experimentsm being already under way.

8. State of the art

Our activity is at the crossroads of advanced ab initio theory and of applications for future all-oxide electronics. We use both conventional (LDA,GGA,GGA+U) and advanced (hybrid, SIC, GW) methods, as

well as free-energy models and semiclassical transport. We work on geometry and electronic structure, optics, magnetism, polarization, transport.

Our first main activity concerns 'visionary' materials concepts of huge basic interest, which may well open unexpected application avenues, for example to high-density multistate memories. Our second main activity is on less adventurous materials, but hardly easier to deal with, namely oxide solid solutions with group III cations, which are currently very rapidly emerging in power electronics and UV optics and sensing.

9. Research description, milestones, and goals

Metallic ferroelectrics

Ferroelectrics are characterized by structural instabilities which, upon condensing, produce permanent dipole moments. A long-standing question which we are tackling is whether such instabilities survive in the presence of free carriers (upon e.g. doping) as the material turns into a degenerate semiconductor or a bad (or a good) metal. We are also progressing on a related but distinct question: is there a single-phase material which is natively ferroelectric *and* natively metallic ? It is difficult to estimate the timeframe of advances in this area, but some preliminary results suggest reasonale chances to obtain an experimentally-verifiable prediction in the short-medium term, hence hopefully an experimental verification within the nd of the 16-18 triennium.

Phase stability of oxide alloys for UV electronics

The semiconducting wide-gap oxides Ga_2O_3 and In_2O_3 are in current focus for UV electronic and sensing, and conductive transparency, respectively, with emerging applications to power electronics. The alloys of these compounds (also including a third ingredient, Al_2O_3) of course allow combining their properties, in principle, at will. Their miscibility at a generic concentration is rather poorly known, since the three binary compounds all have different structures, and of course nothing is known about the preferred structures as function of concentration. Our objective is exploring the phase diagrams of the ternary GaInO (and later GaAlO) alloy with free-energy models where the internal energy is obtained ab initio. Of course this is a long-term work, considering that there exist two to three competing structures just for Ga_2O_3, not to mention the pradigmatically politypic Al_2O_3. In the 16-18 triennium we expect to obtain a reasonably complete, semi-quantitative picture of the phase diagram of the two ternary alloys.

Optical properties and anisotropy in Ga_2O_3 and $(GaInAl)_2O_3$

A typical example of compositionally adjustable properties of semiconductor alloys are optical absorption and emission. As with miscibility, we face the problem that the different cristallographic structures produce different electronic structures, generally complex and not well understood. In Ga_2O_3, for example, it is known that optical absorption is anisotropic, but the reason is not known (we are working on that): the same phenomenon may show up as function of concentration in ternary alloys, and very possibly in a much more complex form. Both the general optical properties and the detailed aspects such as anisotropy, forbidden transitions etc. are an important goal for 2016-18.

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UNIVERSITY of CAGLIARI
Department of Physics

1. Research title
Biological and pharmacological problems approached by computational techniques

2. Principal investigators
Paolo Ruggerone

3. Reasearch team

Full professors	
Associate professors	*Paolo Ruggerone*
Assistant professors	*Andrea Bosin, Giuliano Malloci, Attilio V. Vargiu*
Post-docs	*Giovanni Serra*
PhD students	*Ramaswamy Venkata Krishnan*

4. ERC (European Research Council) classification scheme

PE3_19	LS2_11	PE4_13

5. Keywords

Bacterial resistance	Proteins	Simulations

6. National and international collaborations
Dipartimento di Scienze della Vita e dell'Ambiente, University of Cagliari
Jacobs University, Brema (Germany)
University of Berkeley, Berkeley (USA)
Goethe Universität, Francoforte sul Meno (Germany)
University of Birmingham, Birmingham (UK)
Utrecht University, Utrecht (NL)
Weizmann Institute of Science, Rehovot (Israel)
Université Pierre et Marie Curie - Sorbonne, Paris (F)
Basilea Pharamceutica Ltd., Basilea (Switzerland)
Microbiotix Inc., Worcester (USA)
Angelini Farmaceutica, Pomezia (IT)

7. Abstract
In the next years we will continue the study of bacterial efflux systems, i.e., the proteins involved in the reduction of antimicrobial compounds inside the bacteria, by using a manifold of computational techniques applied to different family of efflux pumps. Additionally, we will extend our database of physic-chemical and dynamical properties of antimicrobial compounds. A new research line will deal with viral proteins that inhibit the action of the immune system. Finally, we will work on a computational protocol that should improve the predictive power of molecular docking.

8. State-of-the-art

The foreseen researches will be performed within the framework of national and international projects and will benefit from a strong interaction with experimental groups: financial support will be provided by two European projects and by the Regione Autonoma della Sardegna.

The continuous increase of bacterial resistance to antibiotics requires a thorough research of the mechanisms developed by the bacteria to survive the therapy. Efflux pumps contribute relevantly to the survival strategy of the bacteria and understanding their functioning at microscopic level provides valuable insights for an efficient design of compounds able to escape and/or to inhibit these efflux systems.

The second research focuses on proteins that are crucial for the extremely dangerous Ebola virus. The goal is to identify possible inhibitors of these proteins starting from the knowledge of microscopic features.

Finally, we will work on the development of a more accurate docking protocol, which is necessary to deal with the problems highlighted just above.

9. Research description, milestones, and goals

In our research activities we use several computational techniques ranging from molecular docking and modeling to molecular dynamics simulations and ab initio methods. Moreover, because of the size and time scales of systems and processes of interest, we will adopt coarse-grained methods to simulate larger systems for longer times keeping the accuracy at a good level. In particular,

<u>Bacterial resistance</u>

Study of the capture, binding, extrusion of selected antimicrobial compounds by the efflux pumps of the RND family in *E. coli* and *P. aeruginosa*. A strong interaction with our industrial partners will offer a strong support to our research (2016-2018).

Simulations of the assembling process of the components of the RND efflux pumps in *E. coli* (2017-2018).

Study of the structural and dynamical properties of the efflux pumps belonging to the MFS and SME families. For such proteins, a synergy with activity of the RND pumps has been suggested (2017-2018).

Setup of database of physic-chemical and dynamical properties of antimicrobial compounds. The database will contain also the files necessary to perform molecular dynamics simulations and the access will be free (2016-2018).

<u>Viral proteins</u>

With extensive molecular dynamics simulations we will identify the residues relevant for the interaction of the protein VP35 with the RNA of the Ebola virus. This interaction is crucial to inhibit the response of the immune system to the virus (2016-2018).

Microscopic characterization of the interaction between the residues identified in the previous point and molecules that can inhibit the formation of the VP35-RNA complex (2017-2018).

<u>Docking protocol</u>

Setup and test of a computational technique to generate protein structure similar to those in complex with ligands starting from experimental apo structures. Additionally, we will use and test site-finder programs that search for putative affinity sites in a protein if experimental data are lacking (2016-2017).

Setup of a relational database containing protein structures available to the scientific community to improve the efficiency and the reliability of docking protocols (2017-2018).

UNIVERSITY of CAGLIARI
Department of Physics

RESEARCH PLAN
Domain “Condensed matter physics”
Sub-domain 02B3 "Applied physics"

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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

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	Synchrotron light

6. National and international collaborations on this topic

INFN SYRMA_CT project: INFN units of TS, PI, CA, NA, FE, BO, Elettra, Azienda Ospedaliera Universitaria Ospedali Riuniti Trieste, Università di Sassari.
INFN AXIOMA project: INFN units of FE, LNL, LNS, NA. PD, PI.

7. Abstract

The research is divided into several sub-projects:
1. Development and application of new dosimetric techniques
2. Techniques for dating of archaeological finds
3. Mammographic tomography with syncrotron light
4. Development of spectroscopy techniques on cold systems for the detection of Cosmological Axions

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. Mammography with synchrotron radiation has two main goals:
   - monochromatic radiation allows a substantial reduction of dose as the low-energy part of the spectrum used in conventional mammography is totally absorbed by the tissues with no contribution to the image formation;
   - the high spatial coherence of the beam makes the effects of phase contrast visible if there is an adequate distance between object and detector. These effects increase the visibility of small details and / or low contrast.

4. We want to study the feasibility of a system for particle detection that exploits the laser-driven, fluorescence-emitting transitions in rare-earth doped crystals (InfraRed Quantum Counter).

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 illumination of the phantom with a parallel beam obtained with a parabolic mirror and focused on a CCD sensor with a similar mirror. 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 has resulted so far in a thesis, a postgraduate Master's thesis and presentations in local congresses.
3. The objective of SYRMA-CT is to maintain the Italian leadership in the mammography phase contrast, extending the clinical program of the SYRMEP line to the breast tomography. The X-ray room, already designed to be compatible with tomography, will be adapted to the new method, as well as the dose control system and the execution control. The project will focus on the dosimetric optimization which is linked to the choice of the energy (in the range 20-34 keV), the spatial resolution of the detector (base spatial resolution is 65 microns), the thickness of the slice (Max 2 mm), the number of tomographic projections. One should be able to use the effects of phase contrast in order to increase the visibility of small details (edge enhancement) or low contrast structures (phase retrievial). The Cagliari group deals with the reconstruction of tomographic images and the optimization of the quality of the image for different acquisition parameters.
4. We foresee to use lanthanide-doped rod as a “coherent” scintillator, based on amplification by stimulated emission, for relatively high energy deposits (for example X-rays or ionizing particles). Development of a coherent scintillator with enhanced time resolution is also useful for applications different from dark matter detection, such as positron emission tomography.

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"

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UNIVERSITY of CAGLIARI
Department of Physics

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

2. Principal investigators
Luciano Burderi

3. Reasearch team

Full professors	***Nicolò D'Amico***
Associate professors	***Luciano Burderi***
Assistant professors	***Alessandro Riggio***
Post-docs	***Andrea Sanna***
PhD students	***Francesca Loi*** ***Sara Loru*** ***Fabiana Scarano***

4. ERC (European Research Council) classification scheme

PE9_10	PE9_11	PE9_13

5. Keywords

High Energy Astrophysics	Radioastronomy	Pulsar

6. National and international collaborations
Dipartimento di Fisica, Università di Palermo
INAF Osservatorio Astronomico di Cagliari
INAF Osservatorio Astronomico di Roma
Universität Erlangen-Nürnberg, Sternwartstraße 7, 96049 Bamberg, Germany
Institut de Cie`ncies de l'Espai (IEEC-CSIC), Barcelona, Spain

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 and Gamma-ray astronomy and observations in the Radio from ground based facilities.

8. 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 294 (to date) 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. This scenario has been very recently confirmed by the discovery of three transitional millisecond pulsars which alternates phases of MSP to phases of Accreting Millisecond Pulsars (AMPs), that is when the X-ray emission due to matter accretion onto the NS is coherently modulated at its spin frequency.

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, and gamma), as well as experts in binary evolution. In particular we plan to perform:

Timing analysis of all future X-ray outburst of AMPs to constrain the orbital and spin parameters and their secular evolution.

X-ray spectral analysis of AMPs in order to constrain the geometry and properties of the emitting region.

Optical observations of AMPs in outburst and, even more intriguing, 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.

Hard and soft gamma-ray observations of AMPs where, using epoch folding techniques together with the extremely accurate parameters derived in 1. could lead to the first pulsation detection of AMPs in the gamma-ray band.

Theoretical modelling of LMXBs, AMPs, 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.

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.

Detection of Gravitational Waves. Within the context of the European Pulsar Timing Array (EPTA) collaboration, we will be deeply involved in an unprecedented experiment, aiming to combine the capabilities of the major european 100m class radio telescopes, including the Sardinia Radio Telescope. 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.

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.

Within the context of the HTRU (High Time Resolution Universe) and SUPERB (SUrvey for Pulsars & Extragalactic Radio Bursts) collaborations, we will carry on an ultra-deep search at the Parkes radio telescope. for additional MSPs and for Fast Radio Bursts (FRBs). 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 AMPs and MSPs.

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.

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.

UNIVERSITY of CAGLIARI
Department of Physics

RESEARCH PLAN
Domain "Analytical and physical chemistry"
Sub-domain 03B1 "Principles of chemistry and inorganic systems"

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UNIVERSITY of CAGLIARI
Department of Physics

1. Research title

Structural characterization and development of antimicrobial peptides and their synthetic analogues.

2. Principal investigators

Prof. Mariano Casu and Dott. Mariano Andrea Scorciapino

3. Reasearch team

Full professors	
Associate professors	*Mariano Casu*
Assistant professors	
Post-docs	
PhD students	*Pira Alessandro e Serra Ilaria*

4. ERC (European Research Council) classification scheme

PE4_13	PE4_1	PE4_3

5. Keywords

Peptidi	Struttura	Spettroscopia

6. National and international collaborations

Prof. Paola Gameiro, Departamento de Química and Bioquímica from Faculdade de Ciências da Universidade do Porto. The experience of this research group will deepen some aspects related to the investigation of the action mechanism of the peptides, such as: study of the lateral mobility of membrane lipids during the interaction with the peptide, determination of the degree of insertion of the peptide membrane, quantitative determination of the constant breakdown of water-lipid-related peptides.

7. Abstract

The research includes the study of the principles underlying the interaction of antimicrobial peptides (AMPs) and cationic phospholipid component of the cytoplasmic membrane of bacteria and fungi, the membrane being a primary objective of the mechanism of the microbicide AMPs.

8. state-of-the-art

Nowadays, bacterial resistance to antibiotics is one of the most pressing public health problems worldwide, and is associated with mortality and high costs. In addition to traditional strengths, now acquired by the vast majority of pathogens, the problem is aggravated by the increase in infections caused by bacteria can form biofilms, following the colonization of surfaces physiological host, eg surgical tools and implantable prostheses, which constitute up to 60% of hospital infections and for which the conventional antibacterial therapies are not effective. At the same time the antibiotic resistance was not compensated by the introduction of new molecules in the arsenal therapeutic, and

it is therefore necessary that alternative strategies place alongside traditional ones to find new drugs antibacterial, urgently required especially for the Gram-negative pathogens.

9. Research description, milestones, and goals

The starting point of the project is the systematic study of different analogues of SB056, a dendrimeric peptide, designed to assess the actual role of the various parameters that characterize the class of these peptides, to reach a deeper understanding of their actual mechanism of action. The study will focus mainly on the determination of the mechanism of interaction peptide / membrane, but the research will be dedicated to the evaluation of the antimicrobial peptides in vitro synthesized from the original. Of these peptides will be carried out in-depth research by combining experimental techniques and modeling to better understand the mechanism of action and function of the various functional units, the tail and the combined peptide. The optimization will have as objectives (i) the length, (ii) and the unsaturations of the tail, (iii) the interchange of loads Lysine and Arginine residues within chains, (iv) the modulation of the net charge of the chains. In particular, fluorescence spectroscopy will be used to collect information concerning the peptide / membrane. The formation of pores, the fusogenic activity and sequestration of anionic lipids, will be designed to distinguish between the possible mechanisms proposed for the General AMP. A study combined NMR / MD will provide details at the atomic level as the structure of the peptide, aggregation, interactions peptide / lipids, the possible inclusion of the peptide in the membrane or any disruption of the membrane, allowing to highlight the mechanism of 'action of these particular molecules and function of the various functional units of the DP, the tail and the chains.
From a scientific point of view, this project allows to highlight the potential applications of dendrimeric peptides with particular regard to their inherent scalability, studies on their structure, organization and guidance in areas of membrane model that will provide essential information on the mechanisms microscopic, the recognition peptide-peptide within the same aspects and fundamental to the understanding of their mechanism of action. These studies will provide to the scientific community a better understanding of the structural and functional characteristics which determine the efficacy and selectivity of these peptides antibacterial / antiviral.

1. Research title

Control of optical properties of functional materials based on d- and f-metal complexes

2. Principal investigators

Paola Deplano

3. Reasearch team

Full professors	*Paola Deplano*
Associate professors	*M. F. Casula*
Assistant professors	*Angela Serpe, Luca Pilia (ric A)*
Post-docs	*Flavia Artizzu, Davide Espa*
PhD students	*Salahudin Attar*

4. ERC (European Research Council) classification scheme

Pe5_9	PE2_9	PE5_6

5. Keywords

UNIVERSITY of CAGLIARI
Department of Physics

Coordination Chemistry	Optics	Organized Molecular materials

6. National and international collaborations

Several international collaborations (A. Cannizzo, Berna; A. Vleck, University of London Queen-Mary College; B. Dietzek, Friedrich Schiller University, Jena, Germany, …) mainly inside COST Action CM1202 "Supramolecular photocatalytic water splitting" Several national (NLO properties: D. Roberto, M. Pizzotti, UNIMI; (Istituto Superiore delle Comunicazioni e delle Tecnologie dell'Informazione); (L. Marchiò UNIPR). Additional cooperations inside the Department.

7. Abstract

The Project is aimed to design&synthesize&process photoactive molecules based on d- and f-metal complexes and to understand how the molecular environment of a photoactive site can be modified in order to tune and control selected light-induced functions such as second order nonlinear optics (NLO), luminescence and photocatalytic activity for hydrogen production from aqueous solvents.

8. state-of-the-art

Currently light-responsive molecular and supra-molecular materials are object of great interest to try to understand the photophysics and photochemistry of complex molecular systems, responsible for energy transfer, charge separation, electron transfer, and isomerization in chromophores interacting with a molecular environment which are capable of replicating naturally occurring systems in both energy storage and signalling. These systems are composed of a chromophore embedded in a non-continuous molecular and complex environment. The environment tunes or changes the response of the chromophore to light absorption in a specific way. In this contest, metal-complexes that may work as switchable second-order NLO-phores, photocatalyst for hydrogen productions from aqueous solvents and luminescent (including NIR-emitting) are particularly appealing due to the availability of versatile, sustainable, and cost-effective routes for the engineering of their chemical and physical properties.

9. Research description, milestones, and goals

The research will be performed in two phases. Phase 1): Preparation and characterization of: a) second order non linear chromophores based on heteroleptic metal d^8-dithiolenes redox or proton NLO-switchable; multinuclear f and d/f metals complexes. Preparation and characterization of luminescent complexes based on metal d^8-homoleptic dithiolenes to be investigated as photocatalysts for hydrogen production from aqueous solutions. Preparation and investigation of luminescent properties of multinuclear lanthanide complexes. Phase 2) The activity will involve the molecular engineering into organized structures of the new molecular species. The NLO-phores will be incorporated and poled, e.g. in the presence of an electric poling and an appropriate thermal treatment, or by self-assembling, in organic or inorganic matrices, or on optical transparent supports. The effect of

chiral substituents on the nano- and crystalline molecular organization and, hence, on the NLO response, will be studied by the Kurtz-Perry technique. NLO measurements are performed at Università di Milano.

Properties of luminescent complexes will be investigated in matrices obtained by sol-gel routes. The ability of this technique to obtain optically clear films and coatings with tunable features will be tested. All-inorganic and organic-inorganic porous matrices will be used.

Photocatalytic properties for hydrogen production are investigated at Institute of Physical Chemistry, Friedrich Schiller University, Jena, Germany, in cooperation with Prof. Benjamin Dietzek.

Expected goals, 1) obtaining: a) complexes with high and/or switchable NLO response; b) complexes with multifunctional properties (e.g. NLO and luminescence); c) complexes as photocatalyst for H_2 production; 2) processing the most promising complexes as thin films and understanding molecular and cooperative aspects able to transform collective molecules in a optically active device.