UNIVERSITÀ DEGLI STUDI DI CAGLIARI

HR EXCELLENCE IN RESEARCH

TITOLO E ABSTRACT TEMA DI RICERCA DOTTORANDI

DEL CORSO DI DOTTORATO DI RICERCA IN

FISICA

XL ciclo

Luca Ferro

Tema di ricerca / Research title:
Charge current neutrino nucleus cross sections and their implications for neutrino and dark matter searches

Abstract:
TBA

Lorenzo Herres

Tema di ricerca / Research title:
Strings, Branes and High Energies

Abstract: String amplitudes in the high energy limit provide a rich and fruitful laboratory in which deep questions about quantum gravity, unitarity and nonlocality can be partially answered. The inclusion of D-branes, nonperturbative extended objects described by the theory, can be exploited to construct, upon supersymmetric compactifications, black-hole solutions in four dimensions. The project's plan is to study dynamically such configurations by probe scattering computations, with the double goal of making contact with supergravity expectations and of going beyond via the inclusion and the interpretation of stringy effects. By suitably tuning the compactification scheme, the D-branes geometrical arrangement in compact space and the nature of the probe state, we will capture many different solutions with a varying amount of supersymmetry from multiple points of view.

Antonio Incollu

Tema di ricerca / Research title:
Il ruolo della plasticità sinaptica nell'apprendimento e nella memoria: dai processi biofisici a livello molecolare alle dinamiche complesse delle reti neurali

Dipartimento di Fisica – Cittadella Universitaria
S.P. Monserrato-Sestu Km. 0.700 – 09042 - MONSERRATO
Amministrazione Tel. 070.675.4702/4704 mail: amm.fisica@dsf.unica.it – www.unica.it

Abstract: L'attività di ricerca mira a indagare il ruolo della plasticità sinaptica nei meccanismi di apprendimento e memoria all'interno del cervello, con un approccio teorico e computazionale multiscala che spazia dalle interazioni a livello molecolare all'emergere di dinamiche complesse in reti neurali di grandi dimensioni. Lo studio combina modelli biofisici dettagliati con descrizioni più astratte a livello *mean field*, con particolare attenzione verso i meccanismi della *working memory*, la cui capacità di mantenere e manipolare informazioni a breve termine anche in presenza di eterogeneità rappresenta un aspetto cruciale della cognizione. In parallelo, il lavoro si estende alla diagnostica per immagini, con lo sviluppo di strumenti computazionali per l'analisi automatica di immagini CT di placche carotidee, responsabili di eventi ischemici cerebrali. L'integrazione tra modellistica neuronale e imaging biomedico mira a far luce sui legami tra danno vascolare periferico e compromissione delle funzioni cognitive.

Lorenzo Orlando

Tema di ricerca / Research title:
Nonlocal Quantum Gravity: Theoretical aspects and Physical implications

Abstract:
TBA

Michela Sestu

Tema di ricerca / Research title:
Elastic and inelastic neutrino and dark matter scattering on nuclei

Abstract:
TBA

Sara Tullio

Tema di ricerca / Research title:
Depleted argon distillation using the Aria facility to search for dark matter in DarkSide-20k

Abstract:
TBA

Nan Zhao

Tema di ricerca / Research title:
Perovskite solar cells

Abstract:

TBA

XXXIX ciclo

Simone Argiolas

Tema di ricerca / Research title:

Towards Molecular Dynamics Simulation of Hybrid Perovskites Crystal Growth

Abstract: Hybrid lead halide perovskites (HLPs) have emerged as one of the most important class of materials in the field of photovoltaics due to their exceptional optoelectronic properties and compositional flexibility. The optimization of chemical methods has allowed the synthesis of HLP semiconductive active layers with state-of-the-art power conversion efficiency above 25%. Yet, the thermal and chemical material instability in operational conditions, the need of large area synthesis and the toxicity of lead cations are still open problems that require alternative strategies to grow high quality films with a precise control of the microstructure at the atomic scale. In this direction, there is an increasing interest in alternative solvent-free synthesis methods such as deposition by thermal evaporation or deposition in ultra-high vacuum by epitaxial growth from molecular beams.

Even in dry conditions, the mechanisms of crystal growth at the atomic scale are not easily accessible by experiments. Theoretical atomistic methods can play an important role in the fundamental understanding crystallization even though large-scale atomistic models (number of atoms N > 1000) and long simulation times (>100 ns) are mandatory. These large models are out-of-reach of accurate *ab-initio* methods because of their high computational cost (scaling with number of atoms as $o(N^3)$). The possible alternative is represented by classical force-fields that make use of physics-based or machine learning interatomic potentials with much lower computational cost that scales linearly with N, so making affordable large-scale simulations at finite temperature and pressure.

In my research project, I will work to the development and numerical implementation the MYP2 model that extend the existing and well-established MYP0 model for MAPI by introducing many-body interatomic terms, leading to a superior description of the structure of clusters and capable to reproduce the spontaneous crystallization from disordered phases. In addition, I will exploit machine-learning models for inorganic CsPbI3 perovskite based on the Atomic Cluster Expansion (ACE) approach with the goal of transfering them to the nanostructures and crystallization phenomena.

Emanuele Domenico Cadeddu

Tema di ricerca / Research title:

Coherent Emitters based on Halide Perovskites Meta-materials

Abstract: Polaritons are quasi-particles formed through the strong light-matter coupling, observable in various types of structures. These polaritons can be harnessed to produce coherent light, with polariton lasing being particularly intriguing because it enables coherent light emission below the typical lasing threshold of a material.

One of the most commonly used structures for studying polariton lasing is metasurfaces. These are periodic photonic structures that, due to their specific architecture, can enhance particular optical resonances. In our project, we will explore methods to generate polariton lasing using metasurfaces.
Hybrid Halide Perovskites (HHPs) have shown remarkable advancements in recent years as materials for photovoltaics and optoelectronics. The interest in HHPs is driven by numerous factors, including their excellent solution processability, high carrier mobility, and tunable band gap, which can be adjusted by varying the chemical composition. Notably, methylammonium lead tribromide ($MAPbBr_3$) is of particular interest due to its strong optical absorption in the visible spectrum, making it a promising candidate for developing polariton lasers.
In my Ph.D. project I will use HHP metasurfaces to create a polariton-based laser.

Nanako Kato

Tema di ricerca / Research title:

Transverse momentum dependent gluon distributions inside the nucleon

Abstract: Protons and neutrons (nucleons) are the building blocks of all atomic nuclei. Their knowledge is essential for understanding various physical phenomena, such as the high energy scattering processes currently under study at the LHC. These are described by the theory of strong interactions (Quantum Chromodynamics) in terms of partons (quarks, antiquarks and gluons), the nucleon's elementary constituents.
Despite significant progress throughout the years, many fundamental questions remain unanswered: where does the mass of the nucleons come from? What contributes to their spin? How are partons distributed inside nucleons?
In my project I will exploit parton distribution functions (PDFs), namely the so-called transverse momentum dependent distributions (TMDs), to access the internal structure of gluons.

Han Kurt

Tema di ricerca / Research title:

Development of a computational protocol to predict protein-ligand complex structures

Abstract: Many aspects of life sciences rely on protein-ligand interactions, which have far-reaching effects on biological research, therapy development like drug design and development, and biotechnology. Understanding these interactions is key to advancing medical, environmental, and technological innovations. In these interactions, the binding of small molecules (ligands) to proteins results in conformational changes, protein structure stabilization, and regulation of biological activity. While laboratory experiments are significant in elucidating protein-ligand interactions, they face limitations due to their high costs, time requirements, challenges in quantification, and the investigation of transient interactions. Because of this, computational *(in silico)* research is necessary for a thorough understanding of binding events at a molecular level, particularly when binding is associated

to significant conformational changes in the protein from the unbound (apo) to the bound (holo) structure. In my project, I will work on the development of a protocol called gEDES - generalized Ensemble Docking with Enhanced sampling of pocket Shape -, which can generate holo-like protein conformations exploiting only apo structures. I aim to validate gEDES against other state-of-the-art methods on about 40 proteins selected from the DUD-e database, a benchmark dataset for docking and virtual screening. In addition, the project's objective is to setup a user-friendly web server that will make it easier for researchers, regardless of their expertise, to set up and run these simulations, as well as to download generated holo-like structures for any available target.

Daniele Provenzano

Tema di ricerca / Research title:

Search for the $\Sigma^+ \to p\, \mu^+ \mu^-$ rare decay and prospects for future studies in the strange physics sector at LHCb

Abstract: Despite its remarkable accomplishments, the Standard Model (SM) continues to be an incomplete framework, leaving various unanswered questions in its wake. For these reasons, one of the main focuses of the particle physics community in the past years has been to search for possible signs of New Physics (NP) beyond the SM. One of the possible approaches to search for new particles is to test the SM predictions with very high accuracy to look for possible contributions from NP particles. In this context, the study of rare and very rare decays, especially of heavy flavours, and of flavour-changing neutral-current processes (FCNC) are a sensitive tool to explore possible interactions beyond those predicted by the SM as can receive possible NP contributions at the same level or even larger than the SM. The Large Hadron Collider beauty (LHCb) experiment at CERN has proven itself to be an ideal setting for this purpose.

During my Ph.D., I will search for the very rare $\Sigma^+ \to p\, \mu^+ \mu^-$ decay at the LHCb experiment will be presented. This decay is an FCNC process, allowed only at loop level in the SM (and thus highly suppressed) and it gained attention in 2005 when the HyperCP collaboration at Fermilab reported the first evidence for this mode consisting of three events with the same dimuon invariant mass leading to the hypothesis that the decay was mediated by an intermediate particle decaying into two muons. The search for this particle in $\Sigma^+ \to p\, \mu^+ \mu^-$ decay had not been repeated prior to the LHCb study using proton-proton collision data recorded by LHCb in 2011–2012 where an excess of events was observed with respect to the background expectation with a signal significance of 4.1 standard deviations and no significant structure was observed in the dimuon invariant mass distribution, in contrast with a previous result from the HyperCP experiment.

Carlotta Sanna

Tema di ricerca / Research title:

Exploring the mid-IR SED of high-mass YSOs

Abstract: Young Massive stars (with masses greater than or equal to 8 solar masses) shape the galaxies at all scales, affecting their formation, evolution and morphology.

However, despite their importance, the processes that lead to their formation are not yet completely understood. The biggest uncertainty comes from the lack of a solid diagnostic tool to classify massive young stellar objects (MYSOs) according to their evolutionary stage. Currently, the only evolutionary indicator for MYSOs, based on a theoretical classification scheme, is the bolometric luminosity to envelope-mass ratio (L/M). Indeed, this ratio changes with evolution, because while the mass of the envelope decreases with time as MYSO uses its mass reservoir, instead the bolometric luminosity increases as MYSO becomes increasingly brighter with its growth. Nevertheless, this method is severely hampered by the extreme extinction of high-mass star forming sites and by the poor resolution of existing facilities in the infrared (IR) regime which limits the accessible scales to those of entire proto-clusters. Indeed, the bolometric luminosity observed is that of the entire cluster, and observationally, very little is known about the spectral energy distribution (SED) of individual MYSOs. Flux measurements of single members of proto-clusters are feasible only at long wavelengths thanks to radio/(sub)mm interferometers.

My PhD thesis proposes a novel approach to investigate the mid-IR properties of single members of proto-clusters through ALMA observations (Atacama Large Millimeter/sub-millimeter Array, which is a millimetric interferometer in the Atacama Desert of Chile). The aim of my project is to develop and test a new method to infer the luminosity of MYSOs on a pilot sample of well-known and characterised massive proto-clusters in different evolutionary phases. My observations target several transitions of different molecules sensitive to the radiation field of MYSOs; in particular, they are reactive to photons emitted between 10 and 45 μm, when the envelope surrounding the protostar reaches and exceeds 100 K. The analysis of these data is crucial to verify that the presence of these transitions is due to a MYSO which has reached a temperature capable of exciting them. The aim is to develop a model to find a unique relation between the intensities of these lines and the corresponding exciting IR field, in order to derive the SED of MYSOs with the excellent resolution of the millimetric interferometer.

Luca Sergi

Tema di ricerca / Research title:

Computational neuroscience: studying structural plasticity mechanisms through firing-rate and spiking models

Abstract: Computational models are essential for understanding the link between high-level cognitive processes and low-level mechanisms involving synaptic changes. These synaptic processes and modifications constitute what is known as synaptic plasticity. There are various forms of plasticity, and structural plasticity is one of the least understood and studied. It involves the stabilization, creation, and deletion of synapses. There is increasing evidence that this form of plasticity plays a critical role in learning and memory consolidation. In this regard, we work on two computational models: a spiking model of the pyramidal cells in the CA1 hippocampal area and a firing-rate-based neuronal network.

The spiking model, based on Poirazi's work, provides a detailed description of the neuron's dynamics, from glutamate concentration to the concentration of filamentous actin (F-actin), a protein critical for synapse formation and the strengthening of existing connections. We have implemented this model in the NEST spiking network simulator, paving the way for future large-scale simulations with detailed neuron dynamics.
On the other hand, we develop a phenomenological computational model that incorporates the effects of structural plasticity in a firing-rate-based neural network. A training-test protocol was employed to ascertain the number of patterns that could be stored by the network. Furthermore, we developed a theoretical framework that enables estimation of the memory capacity of our network as a function of the number of training patterns and other model parameters. This work elucidates the impact of structural plasticity on the memory capacity of a neural network. In the future, such a framework can be used to study the impact of anomalies in structural plasticity, which are postulated to correlate with developmental disorders such as autism and schizophrenia on the learning capability and the memory capacity of a neuronal network.
In summary, our two studies aim to deepen our understanding of the impact of structural plasticity mechanisms in the brain by exploring them across different scales and levels of abstraction, using both firing-rate and spiking neuron models.

Mirko Pitzalis

Tema di ricerca / Research title:

Regular Black Holes and Mimickers: Fundamental Aspects and Observational Implications

Abstract: Einstein's theory of general relativity, to date, is the most reliable theory of gravity. In recent years, the theory has been remarkably confirmed through groundbreaking experimental results, including the first direct detection of gravitational waves by the LIGO and Virgo interferometers. Despite these successes, little significant progress has been made towards a consistent quantum theory of gravity, and the gap in our understanding still represents a major challenge in modern physics. Black holes, some of the most intriguing and exotic solutions predicted by general relativity, are widely believed to offer a crucial window into a quantum theory of gravity, especially because they encompass the regime of strong gravitational fields, where significant deviations from Einstein's classical theory are expected. A consistent theory of quantum gravity is believed to play a crucial role in describing black holes, particularly in regularizing the singularities predicted by general relativity, where the theory's predictive power fails.
Traditionally, it was believed that quantum gravitational effects relevant to the regularization of singular black hole geometries would only become significant at the Planck scale. However, recent theoretical developments suggest that these effects could manifest at scales comparable to the Schwarzschild radius. This has led to the hypothesis that quantum deviations from classical general relativity could introduce an additional parameter, or "hair," representing a length scale that could potentially be measured through experimental observation. This length scale characterizes a new type of object known as

regular black hole or, more generally, black hole mimicker, whose singularity has been regularised. The lack of predictive power at the level of the singularity has therefore led to the intriguing possibility that, in reality, astrophysical black holes might actually be regular objects that mimic the properties of singular black holes. The most compelling hypothesis is that if the hair is sufficiently large, these objects could be regular and have no event horizon. So far, regular models have primarily been found as solutions of general relativity sourced by anisotropic fluids. These fluids are considered an effective description of some yet-to-be-discovered quantum gravity effects, much like how classical fluid dynamics offer a coarse-grained description of the behavior of a large number of atoms and molecules.
In my Ph.D. project I will explore various approaches to using anisotropic fluids to generate regular models within the framework of Einstein gravity minimally coupled to a scalar field. I will investigate viable alternatives to traditional compact objects described by general relativity, focusing on deviations that could be experimentally tested in the near future.

Muhammad Naseem Akhtar

Tema di ricerca / Research title:

Chemical and electrochemical filling of porous silicon for technological applications

Abstract: Porous silicon (PSi) has emerged as a transformative material in modern science and engineering, recognized for its high surface area, tunable pore structure, and compatibility with a wide array of applications, particularly when filled with specialized materials. The inclusion of melanin, nickel, and polyaniline in PSi matrices brings unique characteristics that enhance their applications in various fields like electronics, biomedicine, catalysis and sensing technologies.
Melanin, a naturally occurring biopolymer, increases the absorption coefficient, maintain the PSi biocompatibility and has a good electrical conductivity, making it a suitable candidate for PSi-based biosensor development. If we have become able to control the conductivity of this combination, we can play with the efficiency of solar cells. Polyaniline, a conductive polymer with notable chemical stability, further increases the electrical properties of PSi. This filling is especially effective for electrochemical sensors, offering enhanced performance for environmental monitoring and energy storage applications. Nickel-filled PSi, with its inherent magnetic properties, provides an innovative platform for magnetic sensor applications. This integration yields high-sensitivity sensors capable of detecting minute changes in magnetic fields, proving essential for applications in security, navigation, and bio-magnetic monitoring. Additionally, the unique combination of these fillings allows for precise modulation of the refractive index, expanding the optical utility of PSi in photonic devices and optical sensing. By tailoring the refractive properties, PSi devices can be adapted for specific wavelengths, enabling advancements in optical communication and imaging systems. The multifunctional approach of filling PSi with melanin, nickel, and polyaniline not only broadens its application range but also positions porous silicon as a critical material in the development of next-generation smart materials for electronic, biomedical, and environmental applications. Through this innovative synthesis, porous silicon stands at the forefront of materials science,

ready to contribute to the design of responsive, high-performance systems in diverse technological fields.

XXXVIII ciclo

Simone Anedda

Tema di ricerca / Research title:

TMD effects in inclusive and semi-inclusive hadronic collisions

Abstract: In the context of Quantum Chromodynamics (QCD), the theory of strong interactions, the nucleon is understood as a strongly interacting relativistic bound state composed of quarks and gluons, which are referred to as partons. One approach to treat QCD phenomena involving two energy scales, a large one in perturbative regime and a second soft scale, is the so-called transverse momentum dependent (TMD) approach, in which the intrinsic motion of the partons within the nucleon, and their correlations, are fully taken into account. The need for the TMD framework stems from several failures in interpreting experimental measurements of polarisation observables in strong interactions within the "ordinary" collinear perturbative QCD, where the explicit intrinsic transverse motions of the partons integrated out in first approximation. In order to reconcile theory and experiments, the TMD community is at present focusing on the determination of even better parametrizations of the nonperturbative TMD distributions and fragmentation functions. In my reserch project, I will study azimuthal asymmetries in the production of two almost back-to-back hadrons in two-photon collisions, which are particularly relevant for a better understanding of the fragmentation process and an improved determination of the quark TMD fragmentation functions. I will apply and develop the TMD approach account for the production of colour-neutral final states, such as the lepton pair production in the Drell-Yan process or the Higgs boson production in proton-proton collisions.

Andrea Claudio Maria Bulla

Tema di ricerca / Research title:

Measurements of the electroweak production of two jets in association with a W boson in proton-proton collisions

Abstract: In proton-proton collisions at the CERN Large Hadron Collider (LHC), the pure electroweak production of a lepton-neutrino pair in association with two jets (EW Wjj) includes the vector boson fusion (VBF) channel. This process plays an important role in testing the gauge sector of the Standard Model (SM), in particular, aspects of gauge boson self-interactions. The study of the EW Wjj process is part of a more general investigation of SM VBF and scattering processes that includes searches for physics Beyond the SM (BSM). Many BSM theories have been proposed through the years, with little to no clue on which is the one chosen by nature. The Effective Field Theory (EFT) is a model-independent approach that bridges SM to different BSM theories. The EFT lagrangian is obtained as a generalization of the SM one, where new physics is described as an infinite series of new interaction terms. In my research project, I will perform sensitivity study related to the data collected by the

Compact Muon Solenoid (CMS) during Run-II, with a centre-of-mass energy of 13 TeV and an integrated total luminosity of 137 fb^{-1}.

Camilla De Angelis

Tema di ricerca / Research title:

Λ_0 transverse polarization studies in pNe collisions at $\sqrt{s_{NN}}$= 68.4 GeV at LHCb

Abstract: Transverse polarization of Λ hyperons produced in unpolarized collisions was observed for the first time in 1976 in inclusive production by 300 GeV protons on beryllium target. This was completely unexpected as, at that time, there was an intuitive picture that particle production at high energy would involve a large number of final states, and thus, no polarization would be expected in inclusive production. On the contrary, this experimental observation showed that spin effects played an important role even in high energy physics. Since then, many attempts have been made to explain this effect, both theoretically and experimentally. However, none of these have led to a satisfactory answer.
During my Ph.D, I will study this phenomenon using data obtained in fixed- target collisions at LHC, with the LHCb spectrometer using neon gas target through the SMOG system, the pNe collisions have a centre-of-mass energy of $\sqrt{s_{NN}}$=68.4 GeV. LHCb, in its fixed-target configuration, covers an energy range basically unexplored up to now, creating a bridge between the very high-energy and the low energy collisions.

Francesco Iraci

Tema di ricerca / Research title:

Pulsar Timing Array at low radio-frequencies

Abstract: Pulsars are fast rotating and highly magnetised neutron stars that generate co-rotating beams of radiation and are mostly observable in radio frequency band as periodic sources of emission. They are often referred to as cosmic clocks, since they are very stable rotators and it is possible to predict the arrival time of each pulsar pulse with a precision even below the micro-second. Using an ensemble of the most stable (millisecond) pulsars it is possible to detect the stochastic gravitational waves background through the so-called Pulsar Timing Array (PTA) experiments.
One of the main sources of noise in PTAs (and in turn a limitation to the array's sensitivity to gravitational waves) is the variable dispersive effect induced by plasma on the propagating radio waves. Dispersion is quantified by the column density of free electrons along the line-of-sight (the Dispersion Measure, DM), and it induces a time delay which is inversely proportional to the square of the observing frequency $\Delta t \propto DM/f^2$.

I will study DM variations under multiple frameworks. One focuses on simulations: since in the PTA community there are many methods to estimate DM variations, I will compare those by creating mock datasets which contain all the typical noise components that are usually

present in PTA observations. The aim is to assess which of these methods is performing better.
On the other hand, I will work on real data from two low-frequency European facilities: LOFAR (Low Frequency Array) below 240MHz, and NenuFAR (New Extension in Nançay Upgrading LOFAR) below 100MHz. Since observations from these telescopes will be more sensitive to dispersive delays, I will lead the combination of their data with the most recent EPTA (European Pulsar Timing Array) Data Release 2. This will allow a much better constrain on DM variations effects, as well as an increase of the PTA sensitivity to the detection of the stochastic GW background (currently still below the aimed 5-sigma threshold).

Lorenzo Mirasola

Tema di ricerca / Research title:

Continuous gravitational waves: looking for a tiny signal in a sea of noise

Abstract: Since the first detection of the Gravitational Waves (GW) signal coming from the binary neutron star merger GW170817, and of the associated gamma-ray burst emission in 2017, the LIGO-VIRGO collaboration has entered in the multi-messenger era that opened a new window for observing the Universe. Although the merging of compact objects, such as black holes or neutron stars, has almost become "normal", we are far from having the entire picture. In fact, other three kind of signals are expected to be detected, and, among them, there are the Continuous Waves (CWs).

CWs are persistent signals that are present in the entire run of data taking. The canonical source of CW is a non-axis-symmetric rotating neutron star, which produces a mono-chromatic signal in the source reference frame. CWs have not been detected yet as they have a characteristic amplitude much fainter than the events already found. A plethora of analysis techniques look for these tiny signals exploiting their persistence, hoping to find outliers that cannot be linked to instrumental anomalies. Up to now, no detection has been claimed, although the ongoing run of data taking that will last till late 2024, might give unexpected results.

In my project, I will analyze the CW signal using several specific data analysis techniques.

Francesco Siddi

Tema di ricerca / Research title:

Functionalized TaS_2 for thermoelectric applications: an ab-initio investigation

Abstract: Thermoelectricity (TE) is a very promising field of research where wasted heat is converted into electricity through the Seebeck effect. The TE efficiency is closely connected to the dimensionless figure of merit ZT which depends on the electrical conductivity (σ), the Seebeck coefficient (S) and inversely on the thermal conductivity (k). Therefore, efficient TE materials should have high electrical conductivity and Seebeck coefficient, and low thermal conductivity. In this scenario, many efforts are currently ongoing to optimize zT by increasing S and σ and/or by reducing k. Among different strategies, 2D materials show promising features for TE applications due to their relatively high electronic conduction properties. However, 2D materials still exhibit large thermal conductivities, hindering their possible TE applications. For this reason, great efforts have been recently devoted to reducing their thermal conductivity.

A recent experimental study showed that the 2D TaS_2 functionalization with specific covalently bonded organic sidechains (CBOSs) leads to a drastic thermal conductivity reduction without affecting the electronic properties. However, the role of the CBOSs in affecting k has not fully yet been clarified.

The focus of my work is to investigate this system by proposing a model that comprehensively clarify the reduction of thermal conductivity.

Rui Rui Wu

Tema di ricerca / Research title:

Perovskite single crystal for X-ray detectors

Abstract: In the past decade, metal halide perovskite (HP) has become a superstar semiconductor material due to its great application potential in the photovoltaic and photoelectric fields. In fact, HP initially attracted worldwide attention because of its excellent photovoltaic efficiency. HP and its derivatives also show great promise in X-ray detection due to their strong X-ray absorption, high bulk resistivity, suitable optical bandgap, and compatibility with integrated circuits. Having good temperature stability is crucial for perovskite devices. Of all the perovskite types, the all-inorganic $CsPbBr_3$ and Cs_4PbBr_6 are particularly desirable due to its superior structural stability compared to organic hybrid perovskites. In my research, I will try to grow single crystals that can reach centimeter sizes that can be used to make X-ray detectors, improving sensitivity while reducing detection limits.

Sahar Aghapour Ghourichay

Tema di ricerca / Research title:

New materials for sustainable energy conservation

Abstract: The growing global demand for energy, driven by population growth and urbanization, has emphasized the critical need for sustainable energy solutions. Renewable energy, particularly solar energy conversion, has become a focal area for addressing environmental and energy-related challenges. Photocatalysis offers a promising pathway for harnessing solar energy to produce renewable energy while mitigating environmental issues. Among various photocatalytic materials, graphitic carbon nitride (g-C_3N_4) stands out due to its stability, thermal resilience, chemical inertness, non-toxicity, ease of modification, and notable electrical properties. However, its standalone photocatalytic efficiency is limited by high recombination rates of photogenerated electron-hole pairs. Recent advances have highlighted incorporating carbon-based materials, such as carbon dots, Graphene, Carbon nanotubes, etc., as an effective means to improve charge separation and expose additional active sites, significantly boosting photocatalytic performance.

In my project, I will prepare a novel composite photocatalyst using a rapid and straightforward method by functionalizing carbon nanotubes with polythiophenes and phenyl-modified graphitic carbon nitride. The structural and optical properties of the composite will be analyzed using X-ray diffraction (XRD), transmission electron microscopy (TEM) to examine its morphology and nanoscale features, Raman spectroscopy to assess vibrational characteristics and structural integrity, and UV–Vis spectroscopy to evaluate its optical absorption. Additionally, time-resolved photoluminescence (TRPL) measurements will be performed to investigate the dynamics of photoexcited carriers.

Camilla Guccione

Tema di ricerca / Research title:

Computational insight into small molecules binding to Gastrin-Releasing Peptide Receptor

Abstract: G-Protein Coupled Receptors (GPCRs) are pivotal drug targets, being the largest family of receptor in the human body. Within them, Gastrin-releasing peptide receptor (GRPR) stands out, being implicated in various physiological processes and pathologies including tumors and chronic itch. The only small-molecule known to bind with high affinity to GRPR is PD176252 which, however, presents significant drawbacks preventing its direct usage. Indeed, its rapid degradation and lack of selectivity, hinder therapeutic advancements. To foster the development of more effective treatments based on this compound, we will employ molecular dynamics simulations of GRPR in complex with PD176252, to shed light on its structural and dynamical features. Moreover, we will employ Well-Tempered Metadynamics simulations to explore the receptor-drug binding process at the molecular level. Integration of simulation data with experimental findings will facilitate

the development of tailored treatments for GRPR-associated conditions in oncology and dermatology.

Rouhin Nag

Tema di ricerca / Research title:
Acceleration and Jerk. Getting faster and faster in our search for exotic Binary pulsar systems

Abstract: Pulsars in compact binary systems, especially within globular clusters, present significant challenges for detection due to their complex orbital dynamics. In my project, I employ and compare advanced search techniques, including acceleration and jerk searches, alongside template bank methods, to improve the detection of such exotic systems.

XXXVII ciclo

Mattia Atzori Corona

Tema di ricerca / Research title:

Exploiting CEvNS detectors to constrain new physics

Abstract: The standard model of particle physics has been established to be very successful in describing elementary particles and their interactions, though some inconsistencies exist both experimentally and theoretically. One of the most relevant problem is the so-called (g-2)μ anomaly, namely the long-standing deviation of the experimental determination of the anomalous muon magnetic moment with respect to its theoretical prediction. This could point to a major failure of the standard model and hence to a new paradigm that would be an unexpected breakthrough in particle physics.

In this context, neutrino physics phenomenology in the low-energy regime represents a very suitable probe to shed light on the deepest laws of nature. One of the most profitable tool is coherent elastic neutrino nucleus scattering (CEvNS), theorized by Freedman in 1974. It is a pure weak-neutral-current process that happens when the De-Broglie wavelength of the exchanged Z boson mediator is bigger than the nucleus radius. In this process, the neutrino interacts coherently with the nucleus as a whole, making the cross section some orders of magnitude bigger than that of other low-energy processes that involve neutrinos. Nonetheless, CEvNS has evaded experimental demonstration in the 43 years since its first theoretical description, due to the difficulty in detecting such a low-energy (few keVs) nuclear recoil produced as the single outcome of the interaction.

In fact, the first observation of CEvNS was reported by the COHERENT collaboration only in 2017, which exposed 14.6 kg of cesium-iodide (CsI) scintillating crystals to the neutrino flux produced by a Spallation Neutron Source.

In my research project I will exploit CEvNS to investigating key electroweak and nuclear physics parameters, as the root-mean-square radius of the neutron distribution inside the nucleus, and the so-called weak mixing angle, a key parameter of the electroweak theory of the standard model. I will then show how new physics scenarios, including neutrino electromagnetic properties and new light mediators Z’, can be probed with CEvNS. I will focus on a specific Z’ model capable of solving the (g-2)μ anomaly, presenting the limits on the model that we have obtained using the latest CsI data-set provided by the COHERENT Collaboration in October 2021.

Federica Fabiano

Tema di ricerca / Research title:

ρ Meson Production in Fixed-Target Collision Data at LHCb to Study Quark-Gluon

Abstract: At sufficiently high temperature and energy density, nuclear matter converts to a phase where quarks and gluons are not confined: the Quark-Gluon Plasma (QGP). Such a state is reproduced in the laboratory with ultra-relativistic collisions of heavy nuclei. Indeed, in order to study this particular state of matter, LHCb is developing a unique heavy-ion programme and pioneering the LHC physics extension with its fixed-target mode (SMOG and SMOG2), in parallel to proton-proton measurements.

My research project is based on the ρ meson production in p-Neon collisions at $\sqrt{s_{NN}}=68.6$ GeV as a powerful tool to test the formation of the QGP and improve the knowledge on this deconfined state of matter: this work is preparatory to the main one of my thesis, where the same analysis will be performed with Run 3 p-nucleus and Pb-nucleus data, where higher multiplicities (number of produced particles) are reached and thus higher chances to observe QGP. The other topic I will work on regards the LHCb data acquisition mechanism, which is now based on a fully-software real-time event reconstruction and selection framework. For this reason, it is crucial to monitor the reconstruction performances and improve them by refining the tracking algorithms currently used, in order to reach even higher multiplicities where QGP is expected to be formed. I will contribute to the development of a monitoring tool to map the tracking efficiency at High Level Trigger 2 level of Pb-SMOG2 data in different sub-detectors.

Moulika Hazra

Tema di ricerca / Research title:

Development of novel hybrid photocatalysts for environmental remediation

Abstract: With the increase in industrialization and energy usage in the modern world, the primary focus has shifted to waste management and energy sustainability. For the sustainable development of human society, the development of both pollution-free technologies for environmental remediation and alternative clean energy supplies is an urgent task. Different materials have been discovered to assist in the process of natural degradation of pollutants. Amongst them, semiconductor photocatalysts have received much attention as a potential answer to the problems of worldwide energy shortage and pollution.

We are interested particularly in semiconductor based photocatalysis where the pollutants are transformed into harmless products by the process of light activated redox reaction on the surface of the catalyst. The rigorous studies on this topic worldwide have resulted in the introduction of a large number of semiconductor photocatalysts for the removal of pollutants from the waste water. We plan to find a suitable non-toxic material which can be synthesized at a competitive cost for industrial utilization.

Our aim is to investigate nanoscale semiconductors with the intention of improving their electronic and optical properties and enhancing their photo-response to visible light. Optimization of their reactivity and degree of functionalization, specific surface area, size-dependent properties, etc., using different methods like- self-structural modification and

phase modification by doping (metal and non-metal), noble metal loading, surface sensitization, etc., we plan to improve their photocatalytic behavior and the ability to use sunlight to the maximum potential.

Elisabetta Ladu

Tema di ricerca / Research title:

High-angular resolution studies of water megamasers in Seyfert/LINERs galaxies. The case of the galaxy IC485.

Abstract: Extragalactic water maser sources associated with the Active Galactic Nuclei (AGN), named ‘megamasers’, are unique tools to derive fundamental physical quantities of the host galaxies. Those associated with accretion disks around the supermassive black holes (SMBH) are used to trace the disk geometry, to estimate the BH mass and to measure distances to their host galaxies. Masers associated with radio jets and/or nuclear outflow are used to provide information about the interaction region of the jets/outflow with the interstellar medium. To perform such studies, high angular resolution measurements obtained by the very long baselines interferometry (VLBI) technique are fundamental. So far, albeit with a great scientific potential, only a limited number of water megamasers have been studied into detail. In my research project, I used several observative techniques to investigate (mega)maser sources.

Stefano Lai

Tema di ricerca / Research title:

Lead-free halide double perovskites and perovskites-inspired materials for optoelectronics

Abstract: In the last years, lead-halide perovskite has been one of the most promising materials in the optoelectronic field. Its excellent characteristics such as high light absorption coefficient, low-cost synthesis, low temperature solution process, narrow band emissions, suitable charge carrier lifetime, high photoluminescence quantum yield (PLQY) make perovskite truly attractive in the field of optoelectronic devices. In solar cells applications the power conversion efficiency of perovskite has reached beyond 25%, furthermore, perovskite are promising materials for light emitting diodes, sensors, photoconductor and so on.

Among the manifold type of perovskite, lead-free double perovskites and perovskite-inspired materials are of particular interest due to their enhanced stability in ambient atmospheric conditions, their broadband emission and high photoluminescence quantum yield. Standard formula of double perovskite is A2MIMIIIX6, with A and MI as monovalent cations and MIII as trivalent cation and X6 is typically an halide (I, Cl, Br), or A2MVIX6 while A3MIIIX6 refers to a perovskite-inspired material with lower dimensionality. As the dimensionality decreases, the metal halide octahedra become progressively less connected and the formation of self-trapped excitons (STEs) is promoted.

In my research project I will synthetize these materials in the form of nanoparticles and single crystals and I will characterization their outstanding emission properties by spectroscopic measurements.

Andrea Pierfrancesco Sanna

Tema di ricerca / Research title:

Infrared Properties of Gravity: The Role of the Black-Hole Event Horizon

Abstract: Black holes (BHs) arguably represent the most interesting solution of Einstein's general relativity (GR). They allow testing the theory in the most extreme regime and are an ideal laboratory to investigate possible quantum signatures of gravitational interactions. Although GR represents our current best understanding of gravity, ranging from small to cosmological scales, there are several hints that it is still incomplete. Among them, the so-called singularity problem, namely the unavoidable presence of singularities inside BH cores, where the theory completely loses its predictive power; the lack of a convincing microscopic explanation of the origin of the large BH entropy; the information paradox arising during BH evaporation. The conventional wisdom invokes quantum gravity (QG) corrections to GR at the very small ultraviolet scale (the Planck scale) as a possible resolution to these puzzles. Despite the partial achievements of widely-considered promising candidates, such as string theory or loop quantum gravity, we are still far from having a well-established theory of QG, and, moreover, we still lack a consistent description of the large-scale infrared (IR) physics. It is therefore of theoretical interest to look for possible IR long-range QG effects, namely quantum properties of event horizons in the BH case, as an alternative route to address the abovementioned puzzles. While for a very long time, experimentally probing this regime was a formidable and seemingly unattainable task, the recent detection of gravitational waves (GWs) has opened a promising gateway to such QG effects. Key information regarding BH internal structure or thermodynamics could be contained in the peculiar damped oscillations characterizing perturbed BHs transitioning to their ground state, called quasinormal modes (QNMs), which leave characteristic marks on the observed GW signal.
In my research project I will exploit an effective approach to investigate how the resolution of the singularity problem for a Schwarzschild BH could be related to the presence of long-range QG effects acting at the event-horizon scale. Motivated by recent results in emergent gravity and, specifically, by the analogy with the cosmological Schwarzschild-de Sitter solution, we will construct a broad class of nonsingular, static, asymptotically-flat BH models with a de Sitter core, sourced by an anisotropic fluid, encoding QG corrections parametrized
by a scalar hair. I wll analyze both phenomenological and thermodynamic properties of these models.

Devidutta Gahan

Tema di ricerca / Research title:

Purification of Underground Argon with Aria and Characterization with DArTinArDM experiment

Abstract: The direct search for particles of non-luminous matter component of the universe, i.e. Dark Matter (DM), has been ongoing since few decades and is one of the leading experimental efforts on the global scale in astroparticle physics. The DarkSide-20k (DS-20k), next project of Global Argon Dark Matter Collaboration (GADMC), is planned at Hall-C of LNGS. This is a dual-phase TPC with a fiducial mass of 20 tonnes. Due to the presence of 39Ar, a beta emitter, in the AAr with an activity ~ 1 Bq/kg, we cannot use it in the detector. We can extract Ar stored in underground sources like CO2 wells, called underground argon (UAr), which has 1/1000 of that specific radioactivity. The planned Urania Project in Colorado will extract UAr, which will be then brought to Aria Project in Sardinia (in batches) for cryogenic distillation and to make the argon detector-grade. Samples will be extracted from both Urania and Aria and transported to Laboratorio Subterraneo de Canfranc (LSC), Canfranc, Spain. The characterization of the liquid argon (LAr) will be done with the DArTinArDM project, which is in its test phase underground. The primary aim of this would be to measure the 39Ar activity in each batch of LAr.

Selene Matta

Tema di ricerca / Research title:

Microstructured halide perovskites for energy applications

Abstract: Halogen perovskites represent a family of semiconductors with optical and transport properties that can be widely modified through element substitutions or crystal structure distortions. They are processable in solution and find application in solar cells, LEDs, lasers and detectors. Over the past decade, halide perovskites have shown tremendous potential for next-generation electronic and optoelectronic devices due to their exceptional transport properties. Current studies and, consequently, devices are based on polycrystalline films that present a relatively simple fabrication protocol, while the growth and integration of single-crystal perovskites present significant limitations at present. Nonetheless, presenting a non-rigid crystal structure, this allows it to tolerate large lattice "mismatches" that make it suitable for the formation of heterostructures. Epitaxial heterostructures based on halogen perovskites, in particular, are potentially optimal for device fabrication due to their low defect concentration, exceptional transport properties and high stability.

During my PhD, I will explore the synthesis and characterization of various types of perovskites, with a particular focus on their chemical-crystalline compositions and physical properties. Advanced techniques will be employed to control the quality and thickness of materials, ranging from polycrystalline structures to single crystals, ultimately leading to the creation of a heterostructure between two single crystals with precisely controlled thickness.

Federico Pitzalis

Tema di ricerca / Research title:

Properties and Characterization of new Metal Halide Perovskite

Abstract: Hybrid metal-halide (MHP) perovskites have attracted great interest in the scientific community due to their excellent optical properties, with a wide range of applications, from photovoltaics to light-emitting devices. Hybrid perovskites combine high absorption coefficients and efficient light emission with large nonlinear optical coefficients, strong spin-orbit coupling, ferroelectricity and spontaneous polarization. For such reasons, a research trend is emerging on applying such materials to quantum technologies. One of the early focusses is on circular photogalvanic effect and optical chirality, namely the chiral photonic and chiroptoelectronic effects that transform the photon spin, used to encode quantum information, into an electric signal and viceversa. My research is focused on developing ultrafast optical spectroscopy techniques to investigate structure-property relations in chiral hybrid perovskites.