



# **Manipulation of the entangled quantum degrees of freedom in bulk TMDCs**

**Francesco Cautero**

## **SUMMARY**

The next generation of opto-electronic devices will rely on controlling quantum phenomena at ultrafast timescales, to enable new functionalities. One promising direction is the manipulation of excitonic quasiparticles in low-dimensional materials, such as transition metal dichalcogenides (TMDCs), which exhibit strong light–matter interaction and host tightly bound excitons even at room temperature. To translate these properties into useful device application, it is essential to achieve an ultrafast control of their electronic and excitonic states. In this project, I propose to use advanced instrumentation to pioneer the ultrafast control of exciton properties in TMDCs, contributing to a better design and functionality of future opto-electronic devices.

### **Project description:**

A viable strategy to alter and control the functional properties of complex materials involves driving light-induced phase transition that modifies the underlying electronic landscape. In this context, TMDCs offer a rich playground: their excitonic properties are highly sensitive to changes in lattice symmetry, dielectric environment, and electronic correlations.

Of particular interest are materials where these excitonic responses can be directly probed through both ultrafast optical and photocurrent measurements. Photoconductive switches, when triggered by ultrashort light pulses, provide a powerful method for directly detecting time-resolved charge carrier dynamics with sub-picosecond resolution [1]. By reading out the ultrafast photocurrent response, it is possible to gain direct access to the dynamics of optically excited states, including exciton generation and recombination that alter the conductivity of ultrafast timescales.

This approach opens the path toward understanding and harnessing exciton dynamics for ultrafast switching applications, with potential implications for valleytronic excitonic, or topological opto-electronic devices [2, 3].

With my Master Thesis project conducted at T-ReX at FERMI, I acquired a wide expertise on ultrafast spectroscopies, including Time-Resolved Optical Spectroscopy (TR-OS), that I exploited to gain a direct view on the ultrafast dynamics of the excitons in several TMDC



compounds. Hence, I am already familiar with the basic concepts required for a prompt start of the PhD project.

The first steps of my experimental activities in the PhD course will consist in the use of femtosecond light-pulses to perform pump-probe measurements with tunable pump, from the ultraviolet to the medium-infrared, with the crucial aim of finding the set of parameters (in terms of photon energy and polarization, as well as the sample characteristics) that maximize the optical rotation in few-layer MX<sub>2</sub>-type samples. In order to measure the effect of an ultrafast valley-selective polarization on the electrical conductivity of MX<sub>2</sub> materials, I will optimize and test a new generation of photo-conductive switches. These will allow for an accurate and precise reading of the light-induced conductivity variation, that will find applications also in photovoltaic applications.

Furthermore, to open the door to the study of the functional properties of novel complex materials, I will develop and upgrade the optical setups of the laboratory, adding the possibility to probe the optical properties in the mid-IR energy range. This setup will provide new information on MX<sub>2</sub>-type TMDCs, charge-density-wave and superconducting materials for the second part of my PhD studies.

[1] D. H. Auston et al., Appl. Phys. Lett. 37, 371-373 (1980)

[2] Liu, Y. et al., Nano Res. 12, 2695-2711 (2019)

[3] Jariwala, Deep et al., ACS Nano 8, 2, 1102-1120 (2014)

End of project description.

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Supervisor 1: *Federico Cilento*  
Supervisor 2: *Fulvio Parmigiani*  
Supervisor 3: *Erik Vesselli*

List of courses to be taken:

Title	Teacher	CFU	Hours
Introduction to Density Functional Theory	Peressi/Bidoggia	2	16
Free Electron Laser and Synchrotron based spectroscopies: getting to the nanometer with femtosecond resolution	Masciovecchio	2.5	20
Advanced Spectroscopy of Quantum Materials	Parmigiani	2.5	20
The physics of imaging with X-rays and associated X-ray detectors	Menk/Brombal	3	24
		10	80



# Euclid cluster cosmology with Simulation-Based Inference methods

**Marco Chiarenza**  
**(XLI Ciclo)**

## SUMMARY

*Data-driven approaches using deep learning have emerged as a powerful technique for the extraction of cosmological information from observations of the large-scale structure of the Universe. In particular, simulation-based inference leverages simulations to perform likelihood-free estimation of the probability distributions of the cosmological parameters. In my PhD project, I plan to apply these methods to optimally infer the cosmological parameters from clusters of galaxies from recent surveys, primarily Euclid. This will follow an initial preparation on synthetic catalogues tailored to match the upcoming data releases.*

In the modern theory of cosmology, the dynamics of the Universe is governed by a set of fundamental parameters: the cosmological parameters. These describe the composition of the Universe, the expansion rate, the properties of the initial density fluctuations, and the optical depth to reionization. With this theory, we are able to describe much of the history of our Universe, culminating in the current standard model for cosmology, the  $\Lambda$ CDM one. However, as we are entering the era of precision cosmology, with unprecedented amounts of data coming from current and future galaxy surveys, we need sophisticated and robust methodologies to properly extract the maximum information to either validate or falsify the current  $\Lambda$ CDM paradigm.

In the standard Bayesian approach to statistics, used for most cosmological analyses, the posterior distribution, which describes our knowledge of the unknown parameters given our observations, is obtained from the likelihood and prior distributions by sampling the parameter space using expensive algorithms such as Monte Carlo Markov Chains (MCMC). This method relies on an explicit evaluation of the likelihood that, on most occasions, is too computationally expensive or depends on strong theoretical assumptions necessary to formulate an analytical expression of the likelihood function itself. In addition, instrumental effects and observational systematics can hardly be described analytically. Conversely, through simulations we can in principle fully control the physical process determined by these parameters, and include all these effects and systematics.

Simulation-based inference (SBI, see e.g. [1]), or likelihood-free inference, is emerging as a data-driven alternative approach to Bayesian statistics. It leverages numerous simulations, to be carried out spanning across the parameters' space of interest, to implicitly sample the likelihood and infer the posterior distribution, thus avoiding the need for a direct evaluation.



As part of more recent approaches to SBI, neural networks can be trained on these simulations to perform data compression and learn the mapping from data to the probability density distributions, further improving the inference process and computational speed. In the context of cosmology, both SBI and deep learning algorithms have been extensively investigated in recent years for the study of the large-scale structure of the Universe [2-7].

The focus of this project is to perform SBI of cosmological parameters from large-scale structure survey data primarily coming from Euclid data releases (DR1 and DR2), but also expandable to other surveys at different wavelengths (e.g. eROSITA, SPT-3G). This work will be carried out within the Euclid Consortium<sup>1</sup>. To achieve this, as a first step, I will actively collaborate on the development of a pipeline that post-process halo light cones generated with the code *PINOCCHIO* [8]. These light cones will be enriched with observational systematics that affect clusters' observables (such as photometric uncertainties, projection effects, cluster miscentering, selection functions, survey masks, and baryonic effects) in order to match Euclid DR1 catalogues.

With these realistic mock catalogues, I will train neural networks to perform Neural Density Estimation (NDE), to either directly predict the posterior or to define the form of the likelihood. This step includes a neural data compression to output cluster summary statistics (cluster counts, clustering, and stacked shear profiles [9]) that can be used as inputs in the SBI process. The results will be validated and compared to those of the fiducial Euclid cluster likelihood analysis. In addition, cluster lensing with halo abundance matching [10] can be included in the analysis to relax some galaxy-halo model requirements. The derived posteriors will be complementary to the main analysis of Euclid DR1.

After having proved and validated our initial SBI pipeline, I will investigate more advanced networks that can perform inference directly on the catalogue or at the field level. Graph Neural Networks (GNN, [11-13]) will be trained on the mock catalogues to potentially recover more information than the previous cluster summary statistics, and included in the inference process; due to their nature of handling sparse data as graphs, they are more suited to process complex survey geometries. Furthermore, I plan to explore methods for inferring directly from map-level representations of the Euclid cluster data, which may include the use of Convolutional Neural Networks (CNN) for optimal data compression of the cosmological information [3]. This part of the project will involve applying the previously tested methodologies, which will also include the combination of different probes (clusters, galaxy clustering, cosmic shear), to Euclid's cluster surveys. In principle, the developed methods will be also adaptable to other survey data.

## References:

- [1] K. Cranmer, J. Brehmer and G. Louppe, *The frontier of simulation-based inference*, 2020, Proceedings of the National Academy of Sciences 117, 48 pp. 30055-30062, doi: <https://doi.org/10.1073/pnas.1912789117>
- [2] J. Alsing, B. D. Wandelt and S. Feeney, *Massive optimal data compression and density estimation for scalable, likelihood-free inference in cosmology*, 2018, Monthly Notices of the Royal Astronomical Society 477, 3 pp. 2874-2885, doi: <https://doi.org/10.1093/mnras/sty819>
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<sup>1</sup> <https://www.euclid-ec.org/>



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- [12] P. Villanueva-Domingo and F. Villaescusa-Navarro, *Learning Cosmology and Clustering with Cosmic Graphs*, 2022, The Astrophysical Journal 937, 2 pp. 115, doi: <https://doi.org/10.3847/1538-4357/ac8930>
- [13] J.-Y. Lee and F. Villaescusa-Navarro, *Cosmology with Topological Deep Learning*, 2025, The Astrophysical Journal 989, 1 pp. 47, doi: <https://doi.org/10.3847/1538-4357/ade806>

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Supervisor 1: *Matteo Costanzi*  
 Supervisor 2: *Pierluigi Monaco*  
 Co-supervisor: *Stefano Borgani*

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Formation of cosmic structures	BORGANI / COSTANZI	3	24
Introduction to parallel computing	TORNATORE	3	24
Bayesian Statistics with Numerical Applications	MILOTTI	3	24
Galaxy formation	DE LUCIA	1,5	12
		10,5	84



## Development and testing of a scintillating fiber tracking detector for the MUonE experiment

Susanna Comunello

*The MuonE experiment, under development at CERN, aims at a precision independent determination of the hadronic contribution to the muon anomalous magnetic moment by measuring the elastic  $\mu$ -e scattering at 160 GeV, which demands precise small-angle muon identification; the downstream Muon Filter is pivotal to this goal. This project develops a large-area Muon Filter based on scintillating fiber (SciFi) tracking planes, replacing the 2S silicon modules used in the prototype. The research program foresees the simulation, construction, and beam testing of a SciFi-based Muon Filter, complete with readout electronics and data acquisition, and a holographic monitor for diagnostics.*

The MUonE experiment, under development at CERN, aims at a precision independent determination of the leading order hadronic vacuum-polarization contribution to the muon anomalous magnetic moment through a complementary, space-like approach [1]. The method relies on measuring the running of the electromagnetic coupling at low negative momentum transfer, by reconstructing with high precision the shape of the  $\mu$ -e elastic scattering differential cross section.

MUonE uses a 160 GeV muon beam and consists, in its final form, of a succession of up to 40 independent tracking stations, each equipped with a thin low-Z target followed by an Electromagnetic CALorimeter (ECAL) and a “Muon Filter” (MF) (see Fig. 1). The purpose of this final tracking station is to provide efficient particle identification by tagging penetrating muons, and to supply precise track measurements after the ECAL that can be linked back to the upstream tracks. This is critical in the low scattering angle region, typically below 5 mrad, where the trackers alone do not separate electrons and muons unambiguously.

For the 2025 test run, the MF has been implemented in a “baseline” configuration consisting of two xy tracking planes, each formed by two CMS 2S modules (see Fig. 2). An individual 2S module is composed of two single-sided silicon micro-strip sensor planes, for a total covered area of 10 cm x 10 cm, which provides sufficient geometrical acceptance when positioning the MF downstream of the three-station plus ECAL beamline arrangement used in the test run.

For the final apparatus with 40 stations, the 2S planes in the Muon Filter will be replaced by scintillating fiber tracking planes “SciFi MF”. This proven technology offers a scalable active area and will cover about 51.2 cm x 51.2 cm, matching the larger geometrical acceptance required at the end of the extended MUonE setup. Fig. 3 shows a SciFi Muon Filter prototype.



Once the analysis of the data obtained with the Muon Filter prototype in 2025 is complete, the research program plan is to update the simulations by inserting the model for SciFi detectors in place of the 2S modules. The simulation code uses the MESMER package, which generates muon-electron interactions in the targets, and the FairMUonE software to reconstruct particle tracks after the interaction.

The complete SciFi Muon Filter configuration foresees two pairs of planes, each with orthogonally oriented fibers, mounted on a rigid support with motorized, remotely controllable movements for alignment along the beam. Each plane will be read out by a custom frontend electronic chain producing a stream of digital data, which will be integrated with the main DAQ of the experiment. The entire structure will be housed inside a thermally insulated dark box. The detector will be equipped with a holographic monitor to track any shifts of the tracking planes [2].

The SciFi Muon Filter will be tested at CERN with both muon and electron beams. Beyond commissioning the detector, the goals of the tests are to validate the simulation results and verify integration with the rest of the MUonE apparatus.

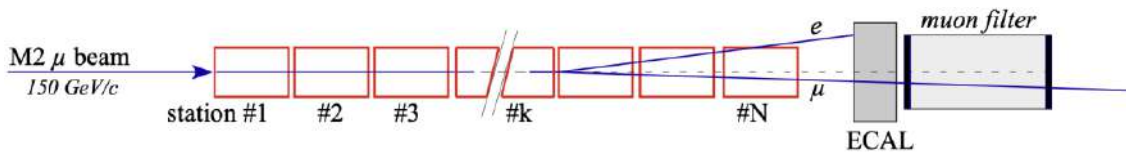


Figure 1 - Schematic representation of the MUonE apparatus.

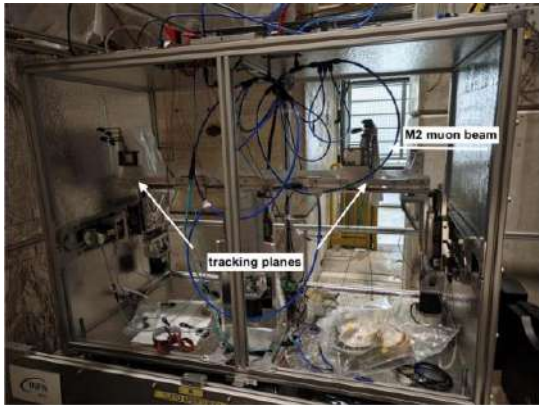


Figure 2 – “Baseline” Muon Filter.



Figure 3 – SciFi Muon Filter prototype.



- [1] G. Hall, , U. Marconi, C. Matteuzzi and D. Pocanic (2024). *Proposal for phase 1 of the MUonE experiment* (CERN-SPSC-2024-015, SPSC-P-370). CERN. <https://cds.cern.ch/record/2896293>.
- [2] A. Arena, G. Cantatore and M. Karuza, "Digital holographic interferometry for particle detector diagnostic," *2022 45th Jubilee International Convention on Information, Communication and Electronic Technology (MIPRO)*, Opatija, Croatia, 2022, pp. 235-237, doi: [10.23919/MIPRO55190.2022.9803636](https://doi.org/10.23919/MIPRO55190.2022.9803636).

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Supervisor 1: *Giovanni Cantatore*  
Supervisor 2: *Francesco Longo*

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Experimental Tests of the Standard Model	Cossutti	2	16
Flavour Physics beyond the Standard Model Concepts and Experimental Techniques	Tonelli/Dorigo	2	16
Simulation of particle interaction	Longo F/Zaccolo	3	24 (16+8)
Advanced data analysis techniques with machine and deep learning	Luparello	2	16
		9	72





# SEARCH FOR DARK SECTOR JETS USING LHC RUN 3 DATA WITH THE ATLAS EXPERIMENT

Giulia Cossutti

## SUMMARY

*This PhD project mainly consists of a search for physics beyond the Standard Model with the ATLAS detector at the Large Hadron Collider, using so-called Emerging Jet signatures, a possible Dark Matter signature at colliders. In parallel, other activities will be carried on within the ATLAS Collaboration, including technical studies on flavour tagging machine learning tools and performance evaluation of the experiment's next inner tracker.*

The aim of this PhD project is to contribute to the analysis searching for Emerging Jets, a possible signature of Beyond Standard Model Physics, using LHC full Run 3 data with the ATLAS detector. The research activity is carried out within the ATLAS Collaboration: therefore, during the PhD, the student will be involved in a number of activities related to the ATLAS experiment. These include technical studies on flavour tagging machine learning tools, to evaluate the impact of the choice of Monte Carlo simulation settings on the tagger's performance and validate it on data, as well as contributions to the ATLAS detector data-taking and upgrade operations, particularly focusing on the quality control tests of the new ITk tracker silicon pixel modules.

Some theories built to explain the nature of Dark Matter hypothesise the existence of a sector of particles beyond the Standard Model, referred to as Dark Sector. In analogy with the Standard Model, Dark Quarks and Gluons would interact through a Dark QCD-like interaction with  $SU(N)$  symmetry. The communication between the Standard and the Dark Sector would be given by a *portal*, a particle field coupled to both sectors [1][2]. Several hypotheses have been made about the portal: it could be a new massive scalar  $\phi$ , a vector  $Z'$  boson or the SM Higgs boson [3]. At colliders, Dark Quarks could be produced through portals in hadronic or leptonic collisions, hence beginning partonic showers and hadronising into Dark Sector hadrons, forming Dark Jets. Depending on their mean life and their probability to decay into visible Standard Model particles, Dark Jets could produce Fully-Invisible, Semi-Visible, or Emerging Jets final states.

The ATLAS [4][5][6] and CMS [7][8] experiments at the LHC have been searching for Dark Jets produced through a new scalar or  $Z'$  portal in the last years. In particular, the last ATLAS search for Emerging Jets through a  $Z'$  portal [6] uses  $51.8 \text{ fb}^{-1}$  Run 3 data.

This analysis aims to search for Emerging Jets coming from various portals using full Run 3 data. By 2025,  $301 \text{ fb}^{-1}$  integrated luminosity data were recorded by ATLAS, and the projections predict the LHC to deliver another  $50 \text{ fb}^{-1}$  to the experiment until the end of Run 3 in 2026. The larger amount of statistics would hence improve the measurement in [6] by reducing the current exclusion limits on cross sections by nearly 60%.



To improve the Emerging Jet tagging, part of this PhD work would consist of developing and training more efficient machine learning tools, for instance, using the new ATLAS GN3 Graph Neural Network. The plan is to interface the new tagger to the ATLAS Reconstruction software. This could also improve the experiment's flavour tagging techniques, to which Dark Jet tagging is strongly linked, and be useful to other ATLAS analyses looking for Emerging and Semi-Visible Jet signatures.

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- [2] T. Cohen et al., "LHC searches for dark sector showers," JHEP, 2017, 11. [link](#)
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- [8] CMS Coll., "Search for dark QCD with emerging jets in proton-proton collisions at  $\sqrt{s} = 13$  TeV," JHEP, 2024, 7, 142. [link](#)

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Supervisor 1: *Michele Pinamonti*

Supervisor 2: *Giancarlo Panizzo*

Supervisor 3: *Paolo Camerini*

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Dark Sector Experiments and Physics Beyond the Standard Model	CANTATORE	1	8
Advanced data analysis techniques with machine and deep learning	LUPARELLO	2	16
Introduction to RooFit	PINAMONTI	2	16
Ionising particle detectors. Gas detectors. RICH detectors	DALLA TORRE	2	16
Flavour Physics beyond the Standard Model Concepts and Experimental Techniques	TONELLI/DORIGO	2	16
		9	72



## Blips and other glitches: characterization and identification Fabrizio Diaz Guerra

### SUMMARY

*Gravitational wave interferometers are affected by many kinds of noise. The category that is more difficult to deal with is transient noise, that can mimic physical signals. Investigating the multiple origins of this kind of noise, modeling the expected signals and finding methods to discriminate between noise and astrophysical signals is a key part of the data validation process.*

This PhD project finds its direct application in the detector characterization of the Virgo experiment.

Many kinds of noise afflict the detector: there are stationary, Gaussian noises that range from terrestrial to thermal noise; but there also are transient noises.

The latter, often called glitches, have multiple origins: from unwanted light scattering inside the system, to low-flying aircrafts. In my master thesis, I investigated a possible origin for a yet unexplained class of glitches. This class, which includes glitches until now distributed in the categories of “blips”, “repeating blips”, “tomtes”, and “koi-fish”, may be a form of “crackling noise”. Crackling noise is a phenomenon associated with forces driving complex systems, where the response of such systems involves a chaotic component that gives birth to what we call noise. In my master thesis, I elaborated algorithms capable of simulating the random component that we associate with noise transients. The basic model depends on two parameters that need to be estimated from real noise data.

My PhD project will extend my previous work in multiple directions. A part of it will consist in the identification of possible physical sources of crackling noise in the LIGO and Virgo gravitational-wave interferometers. Another part of the project will include the correct definition of this class of glitches, separating them from other kinds of transients, and using the resulting dataset to fix the parameters of my simulations.

This project could be extended to include the modeling and simulation of other classes of glitches originating from other physical phenomena. Having a clear model for all kinds of glitches is important to build synthetic glitch datasets, that can find many uses. One of them is the study of subthreshold events contribution to noise estimation, important to assess the statistical significance of astrophysical events. Another important use of synthetic glitch datasets is the training of neural networks as discriminators between astrophysical and noise signals; a process that now finds limitation in the small set of real validated glitches, insufficient to the large needs of those algorithms.

Supervisor 1: *Edoardo Milotti*

Supervisor 2: *Agata Trovato*



List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Bayesian Statistics with Numerical Applications	Milotti	3	24
Advanced data analysis techniques with machine and deep learning	Luparello	2	16
Introduction to parallel computing	Tornatore	3	24
		8	64



# DEVELOPMENT OF THEORETICAL MODELS AND ACQUISITION TECHNIQUES FOR PHASE-CONTRAST TOMOGRAPHY

**Marcello Fonda**

## SUMMARY

*Modern X-ray imaging reveals fine internal structures by using absorption, refraction and scattering, but it works best with the monochromatic beams available at synchrotrons. Laboratory sources emit a broad range of energies, causing distortions that limit image quality. This project develops models that describe how mixed-energy X-rays interact with matter and uses them to improve reconstruction methods. The aim is to reduce artefacts and bring laboratory imaging closer to synchrotron-level performance.*

Phase-contrast X-ray imaging has become one of the most advanced approaches for visualizing the internal structure of samples in fields such as medical physics, histology, materials science, and archaeology. Unlike conventional absorption-based imaging, these methods make use of refraction and scattering effects, which reveal subtle variations inside the material. However, most existing models assume X-ray beams that are both monochromatic and highly coherent, conditions typically met only at synchrotron facilities. Laboratory sources, although increasingly powerful, emit a broad range of energies. This produces image distortions related to dispersion and beam hardening, which are not fully captured by current theoretical frameworks.

The project aims to generalize phase-contrast reconstruction methods so that they correctly describe the interaction between a polychromatic beam and the sample. The strategy is to exploit the redundancy of the acquired data and incorporate energy-dependent effects directly into the forward and inverse models. By doing so, the approach will make it possible to obtain sharp, reliable, and artefact-free images even when working with mixed-energy laboratory sources. Ultimately, this will allow tabletop systems to approach the quality of imaging traditionally associated with synchrotron beamlines.

The work will begin by modelling the propagation of X-rays through the sample using wave-optical descriptions based on the Fresnel propagator, as well as complementary ray-based formalisms. These models will be combined with the true emission spectrum of the source and with the mathematical description of tomographic projection. Two parallel development paths will be pursued. The first is a semi-analytical approach, in which controlled approximations—such as paraxial assumptions and power-series expansions—will be used to derive simplified but accurate expressions for image formation. The second is a numerical approach, in which a more complete physical model is kept and solved

through numerical optimization methods, allowing explicit inclusion of scattering, dispersion, and beam-hardening effects.

To evaluate performance, the theoretical models will be tested through numerical simulations on digital phantoms with known absorption and refraction properties. A Python-based framework will be developed and used to simulate propagation, incorporate the polychromatic spectrum, add noise, and perform reconstruction through gradient-based optimization. The quality of each approach will be assessed in terms of reconstruction error, contrast, noise behaviour, computation time, and resource requirements.

The experimental work will be carried out at the OptimaTo laboratory of the University of Trieste, in collaboration with Elettra Synchrotron Trieste. Measurements with polychromatic laboratory sources will be compared with synchrotron-based data obtained through beam-time proposals at European facilities such as ESRF and PSI. This combination of theoretical development, simulation, and experimental validation will provide a solid foundation for next-generation phase-contrast tomography with widely accessible X-ray sources.

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Supervisor 1: *Pierre Thibault*

Supervisor 2: *Luca Brombal*

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
The physics of imaging with X-rays and associated X-ray detectors	MENK/BROMBAL	3	24
Advanced data analysis techniques with machine and deep learning	LUPARELLO	2	16
Imaging with X-rays - fundamentals and applications	THIBAUT/DI TRAPANI	2	16
Bayesian Statistics with Numerical Applications	MILOTTI	3	24
		10	80





# SYNTHESIS AND CHARACTERIZATION OF MODEL FUNCTIONAL 2D MATERIALS: A BIOMIMETIC APPROACH TO THE ENERGY SUPPLY CHAIN

Simone Formentin

## SUMMARY

*Addressing environmental challenges requires new sustainable and efficient technologies. In this context, bidimensional metal–organic materials represent novel promising systems for efficient heterogeneous catalysis. My PhD project focuses on the growth and characterization of such layers in order to investigate the microscopic mechanisms governing key energy-related reactions, including hydrogen production, conversion and storage, CO<sub>2</sub> activation and ammonia synthesis.*

Project description, around one page. You can insert pictures and reference

### Motivations:

Developing novel, sustainable and cost-effective technologies to address environmental challenges is one of the central goals of modern society. In this context, bidimensional (2D) metal-organic materials (the 2D counterpart of metal-organic frameworks, for which Kitagawa, Robson and Yaghi were awarded the Nobel Prize in Chemistry in 2025) represent promising candidates for heterogeneous catalysis<sup>[1,2]</sup>. Their remarkable properties arise from the possibility to tailor their electronic and chemical structure, and therefore their catalytic activity, down to the molecular level, as well as from the unique effects induced by the quantum confinement of electrons in nanostructured systems. This versatility makes 2D metal-organic networks particularly attractive for the efficient catalysis of key industrial and energy-related processes, such as hydrogen production, conversion and storage. In this perspective, a specifically challenging reaction is represented by ammonia synthesis, which is commonly performed via the energy-demanding Haber-Bosch process, which led both Haber and Bosch to be awarded Nobel prizes in Chemistry for the synthesis of ammonia and its industrial production. When designing new metal-organic networks, scientists can take direct inspiration from nature by adopting a biomimetic approach, by engineering, tailoring and configuring metal-organic layers in order to mimic the active sites of natural enzymes. The latter catalyze fundamental biological processes such as molecular transport, light harvesting and molecular synthesis and conversion<sup>[3–5]</sup>. Enzymes active sites typically comprise small reaction centers (clusters) or even single metal atoms stabilized within an organic scaffold. The catalytic activity of the active sites is determined by their electronic configuration and chemical



environment, which are modulated by the proximal ligands of the metal site, i.e. the first coordination sphere, and by the surrounding organic environment, i.e. the second coordination sphere<sup>[6]</sup>. In the design of 2D metal-organic networks, these structural and electronic properties can be reproduced by co-depositing single metal atoms or clusters and organic ligands onto suitable supporting substrates, following self-assembly into ordered architectures. The support itself plays a crucial role, influencing the system's catalytic performance through the interaction with the organic layer.

### **Techniques and goals:**

Over the next three years, my research will focus on the growth and characterization of 2D biomimetic self-assembled metal-organic layers on different substrates, including Gr/Ir(111), Au(111) and Al<sub>2</sub>O<sub>3</sub>/NiAl(111). The objective is to investigate the chemical and physical mechanisms underlying key reactions in energy-related processes, such as the oxygen reduction and evolution reactions, which are central to the design of new bi-functional electrodes for metal-air rechargeable batteries, as well as hydrogen synthesis, conversion and storage, CO<sub>2</sub> activation and conversion, and N<sub>2</sub> fixation at room temperature for ammonia synthesis.

The starting molecular building blocks will include functionalized porphyrins, synthesized ad hoc in order to reproduce the first and second coordination spheres of natural enzymes, as well as thiophenes and other sulfur-containing aromatic molecules. The growth of these layers will be carried out under Ultra-High Vacuum (UHV) conditions using deposition techniques such as Physical Vapor Deposition (PVD) by sublimation and Electrospray Ionization Beam Deposition (ESIBD).

The metal-organic layers will be characterized under both UHV and Near-Ambient Pressure (NAP) conditions using a combination of microscopic and spectroscopic techniques, including Sum Frequency Generation (SFG) spectroscopy, Near-Edge X-Ray Absorption Fine Structure (NEXAFS) spectroscopy, X-Ray Photoelectron Spectroscopy (XPS) and Near-Ambient Pressure XPS (NAP-XPS).

### **Schedule:**

During the first year of my PhD, I will focus on optimizing the growth of the metal-organic layers by exploring the most suitable deposition techniques for each molecular tecton. In parallel, I will take part in the technical improvement of our laboratory's experimental setup, including upgrades in the design of the measurement cell and the implementation of a new control software for improved sample handling and laser alignment.

The second and third years will primarily focus on the characterization of the metal-organic layers using the different techniques described above. My activity will also include the writing of research proposals to access synchrotron radiation facilities, allowing us to exploit various synchrotron-based techniques such as XPS and NEXAFS spectroscopy, which will yield essential insights into the chemistry and structure of our systems.

End of project description.



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- [2] D. Li, A. Yadav, H. Zhou, K. Roy, P. Thanasekaran, C. Lee, *Glob. Chall.* **2024**, *8*, 2300244.
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- [6] M. Zhao, H.-B. Wang, L.-N. Ji, Z.-W. Mao, *Chem. Soc. Rev.* **2013**, *42*, 8360.
- 

Supervisor 1: *Erik Vesselli*

Supervisor 2: *Nicola Seriani*

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Free Electron Laser and Synchrotron based spectroscopies: getting to the nanometer with femtosecond resolution	Masciovecchio	2,5	20
X-ray photoelectron spectroscopy	Baraldi	1	8
Scanning Probe Microscopies	Africh	1	8
Nanostructures in Catalysis	Fornasiero	1	8
X-ray Absorption Spectroscopy	Bignardi	1	8
Valence Band and Angle Resolved Photoemission Spectroscopy ARPES	Petaccia	1	8
Introduction to Density Functional Theory	Peressi/Bidoggia	2	16
		9,5	76



# **Design and Implementation of an Active Optics KB Mirror System for Next-Generation Free Electron Lasers and Diffraction Limited Storage Rings**

**Nicholas Goldring**

## **SUMMARY**

Over the past decade, new light sources such as free-electron lasers and upgraded synchrotrons have revolutionized research by producing extremely bright and short light pulses. These advances demand more precise and durable optical systems to guide and focus the beams. This PhD project focuses on improving the KAOS mirror system, originally developed at FERMI, so it can handle the higher power and tighter performance requirements of next-generation light sources. The work will combine mechanical and thermal modeling with wave-optics simulations to predict how mirror design and heat affect beam quality. Results from experiments and surface-shape measurements will be used to refine both the models and the hardware, creating a unified design and testing process for future high-performance optical systems.

Project description, around one page. You can insert pictures and reference

Over the past decade, the landscape of light sources has undergone a profound transformation. The advent of free-electron lasers (FELs) delivered to users ultrabright, ultrashort pulses on the order of 100-10 fs, enabling unprecedented experiments across many disciplines. Concurrently, synchrotron facilities have embarked on extensive upgrade campaigns, migrating toward diffraction-limited storage rings (DLSRs) to achieve source brilliance previously thought unattainable. This momentum has been matched by the emergence of new light facilities worldwide—most notably SHINE in China and the EUPRAXIA electron-plasma accelerator project in Europe—alongside next-generation FEL upgrades such as FERMI 2, which push both wavelength reach and temporal resolution further.

Against this backdrop of evolving source capabilities, the demand for high-performance optical systems has never been greater. Optical solutions that proved robust and reliable during the “first phase” of FEL life now serve as crucial foundations for novel designs. Lessons learned from those early implementations—centered on mechanical stability, alignment flexibility, and cost-effective fabrication—, and refined in years of use and study, are indispensable for meeting the stringent requirements of tomorrow’s light facilities.

In this context, KAOS (the KB Active Optical System) emerged as a groundbreaking platform. Originally conceived at FERMI to operate over the 70 nm–4 nm range, KAOS



has demonstrated exceptional versatility, reliability, and cost efficiency. Its modular design and active control strategy have enabled the system to simultaneously power three beamlines at the FLASH facility, validating its performance under demanding conditions.

Widespread interest in the KAOS system from the FEL community has motivated the creators of the system to upgrade the architecture to accommodate next-generation FELs operating at higher repetition rates and photon energies. New FEL facilities, operating at shorter wavelengths, will also see lower grazing angles thereby requiring longer mirrors to capture the full beam footprint. In addition to new FEL facilities, such as FERMI 2, the KAOS system will be useful to and has attracted interest from DLSRs such as the imminent Elettra 2.0 synchrotron.

The objective of this PhD project is to improve the KAOS system to meet the challenges and demands of next-generation FELs. This will specifically involve two aspects: scaling the mechanical design and developing an efficient cooling scheme to manage the high heat loads expected in these facilities, similar to those already observed in DLSRs.

This project will implement a workflow that integrates finite element analysis (FEA) simulations—modeling the mechanical response of the system—with wave-optics simulations. The wave-optics stage will use the FEA output to compute the diffracted spot, thus enabling us to assess the focusing system's performance. Specific investigation directions include: scaling up the mechanical design; developing new or longer mirror geometries; studying mirror tapering; and evaluating thermal-load effects as a function of wavelength. Commercial codes such as COMSOL, ANSYS and ANSYS Fluent will be employed for mechanical and thermal simulations. The community codes WISER and SRW will be used for full physical optics (i.e. wave-front propagation) simulation and ultimate assessment of optical performance. Additionally, this project will seek to elucidate methods for accurately calculating interaction between the power densities produced in a variety of FEL systems (taking into account source characteristics, photon wavelength, beam size, and divergence) and the optical devices under development.

Finally, whenever possible, a practical metrological check will be conducted in order to assess the validity of mechanical prototypes developed in tandem with the simulation workflow outlined above. Figure-error profiles (deviation between ideal and as-built surface) will be obtained using the long trace profiler at the Elettra Optical Metrology Laboratory; in turn, these profiles will serve as inputs for the wave-optics simulations which will in turn be used to gauge the overall performance of the simulated system. Metrology here serves a dual purpose: 1. Aid in the specific development of new KAOS models. 2. Establish an iterative, integrated workflow, that combines numerical simulation and mechanical prototyping.

End of project description.

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Supervisor 1: *Fulvia Arfelli*

Supervisor 2: *Matteo Altissimo*

Supervisor 3: *Alberto Simonci*

Supervisor 4: *Pierre Thibault*

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Principles of Free-Electron laser physics	GIANNESSI	2	16
Introduction to parallel computing	TORNATORE	3	24
Advanced data analysis techniques with machine and deep learning	LUPARELLO	2	16
The physics of imaging with X-rays and associated X-ray detectors	MENK/BROMBAL	3	24
		10	80





# PROBING CLASSICAL GRAVITY VIA DIFFUSIVE SIGNATURES: A QUANTUM INFORMATION APPROACH

**Giorgia Infantino**

## SUMMARY

*This project aims to develop a theoretical framework that, based on the hypothesis that the gravitational interaction satisfies the principles commonly known as Local Operations and Classical Communication (LOCC), investigates the implications of this assumption. The main goal is to exploit quantum information tools to explore the signatures of an LOCC gravity, such as the presence of diffusive dynamical effects in the system, thus testing the possibility of a classical nature of gravity.*

## Scientific context and state of the art

Within the ongoing debate about whether gravity is a quantum or classical phenomenon, theoretical proposals based on *gravitationally induced entanglement* have opened the way to indirect tests of gravity non-classicality [1]. The main drawback of such class of proposals is that they require the manipulation of macroscopic quantum states, which remains beyond the reach of current technology. It is therefore of great interest to identify alternative strategies that can reduce the complexity of the systems involved and the high degree of quantum control required. In this regard, some recent suggestions [2, 3] offer an alternative approach to the problem. They explore the physical implications of assuming that gravity effectively acts as a LOCC mechanism, thus inherently classical and incapable of generating quantum correlations between two masses, and look at the consequences of this classicality in the system. The predictions derived from this assumption do not require the creation of macroscopic quantum states and are thus accessible with existing technologies such as advanced optomechanical systems [4,5].

## Core of the proposal

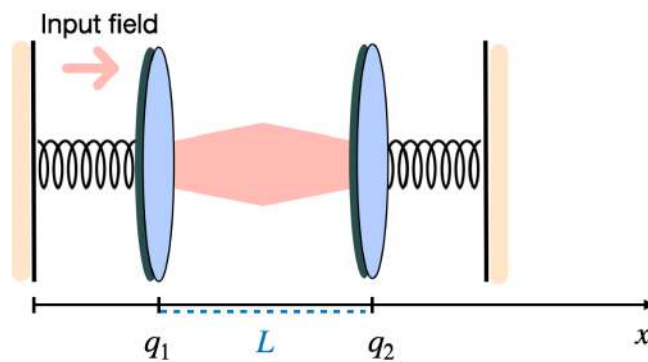
If gravity acts as a LOCC, it should induce a diffusive dynamic in the system [2], which can serve as an operationally detectable signature of its classical nature. However, testing these diffusive dynamics still presents its challenges as the expected signal is extremely weak and therefore difficult to detect. This project looks at the possibility to apply tools from Quantum Metrology and Quantum Information fields to identify optimal experimental setups and detection techniques for such effects. In particular, the interest of applying quantum metrology, is to determine

fundamental bounds on “classicality” parameters, such as diffusion, and to design optimal measurement setups and strategies that maximize the extractable information [7].

Another point which is thought to be interesting to explore is the use of *Quantum Hypothesis Testing (QHT)* which might be able to provide a rigorous framework for discriminating between alternative physical models, allowing one to assess the significance of a given simulation [4, 6]. Hypothesis Testing, in fact, is a statistical method designed to discriminate between two hypotheses, which we may label as a positive and negative outcome, by minimizing the so-called error probability, i.e. the probability of making a mistake when inferring one the two possible outcomes. In contrast with its classical counterpart, QHT leverages quantum resources, offering enhanced discrimination power.

Finally, another key idea of the project regards the application of such techniques in the context of optomechanical systems, which represent a promising experimental platform for simulating and testing weak gravitational interactions.

Among the main advantages of such systems there are high level of quantum control over mechanical degrees of freedom, excellent metrological sensitivity, and flexibility with respect to different experimental protocols [4,5].



**Fig.1:** simple example sketch of an optomechanical platform designed to probe gravitational effects. A Fabri-Perot cavity with two movable mirrors, modelled as massive mechanical oscillators, is coupled with an optical intracavity mode, whose resonance frequency depends on the mirror separation.

## Project development

The first six months will be devoted to a detailed review of the literature related to the LOCC gravity hypothesis, as well as the completion of the doctoral coursework as required by the program.

The following two years will focus on the core research activities, with the main milestones being:



- Modeling of diffusive channels associated with gravitational dynamics of the system,
  - Analytical study of noisy Gaussian systems,
  - Calculation of fundamental metrological bounds on the estimation of diffusion parameters,
  - Design of optomechanical setups and assessment of their experimental feasibility.
- The final six months of the PhD will be dedicated to finalizing the scientific papers and writing the dissertation.

## Conclusions

On the whole, as the question of whether gravity is classical or quantum in nature remains an open and deeply compelling problem, the objective of this project is to contribute actively to this debate by providing a theoretical toolkit and concrete proposals for the detectability of phenomena arising from the interaction between classical gravity and quantum matter.

## Bibliography

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- [2] Angeli, O., Donadi, S., Di Bartolomeo, G., Gaona-Reyes, J. L., Vinante, A., & Bassi, A. (2025). *Probing the quantum nature of gravity through classical diffusion*. arXiv:2501.13030 [quant-ph].
- [3] Lami, L., Pedernales, J. S., & Plenio, M. B. (2024). *Testing the quantumness of gravity without entanglement*. Physical Review X, 14, 021022.
- [4] Marchese, M. M., Belenchia, A., Pirandola, S., & Paternostro, M. (2021). *An optomechanical platform for quantum hypothesis testing for collapse models*. New Journal of Physics, 23, 043022.
- [5] Aspelmeyer, M., Kippenberg, T. J., & Marquardt, F. (2014). *Cavity optomechanics*. Reviews of Modern Physics, 86, 1391–1452.
- [6] Helstrom, C. W., Fry, D. W., Costrell, L., & Kandiah, K. (1968). *Statistical theory of signal detection*. Franklin Book Co.
- [7] Seveso, L., Rossi, M. A. C., & Paris, M. G. A. (2017). *Quantum metrology beyond the quantum Cramér–Rao theorem*. Physical Review A, 95, 012111.

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Supervisor 1: *Angelo Bassi*

Supervisor 2: *Mauro Paternostro*



List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Modern experiments in quantum optics and quantum information	BRUNO / SCAZZA / MARINELLI	1	8
Decoherence in Open Quantum Systems	CARLESSO	2	16
Advanced quantum mechanics and selected applications to quantum computation	DONADI	1,5	12
Complete positivity in quantum information	BENATTI	2	16
Advanced topics in quantum information	MARZOLINO	2	16
		8,5	68



# ATOM-PHOTON ENTANGLEMENT WITH TIME-BIN ENCODING AT TELECOM WAVELENGTHS

## Christian Kodarin

### SUMMARY

*Design and realisation of a quantum interconnect with a neutral-atoms-based architecture. The experiment leverages the properties of cavity quantum electrodynamics for the production of atom-photon entangled pairs. Combining a high-finesse optical cavity with the accurate control given by reconfigurable arrays of optical tweezers and a continuously-operating architecture will lead to ground-breaking performances in quantum communication for both quantum networks and modular quantum computing.*

Quantum networks represent a powerful tool not only to establish fast and secure communication, but also for non-local quantum sensing and modular quantum computation, where multiple interconnected quantum processors collaborate to tackle problems that would be unsolvable with a classical approach. The infrastructure connecting the quantum computing units in a quantum network is called a quantum interconnect.

Currently the scalability of quantum networks is hindered by key challenges such as: limited rate of operation due to the stochasticity of the entanglement process between distant modules, and inefficient exchange of information over long distances due to exponentially increasing loss probability of mediators.

Among many candidates, neutral atoms in optical tweezers and optical lattices are a leading platform to explore scalability of quantum systems, showing long coherence times, fast gate operations, and the potential to manipulate thousands of qubits simultaneously. Among these, 171-Yb stands out for its rich internal structure allowing for the simultaneous encoding of two qubits in a single atom exploiting the  $1S_0$  and the  $3P_0$   $F=1/2$  two-states manifolds [N. Chen et al., Phys. Rev. A 105, 052438 (2022)].

This PhD project aims to design and construct a modular experimental platform that allows fast continuous operation of a quantum interconnect, which could become a node in a quantum network. The ability to generate atom-photon entangled pairs is vital for this purpose.

Ytterbium intercombination line  $1S_0 \leftrightarrow 3P_1$  at 556 nm can be exploited for this purpose for modular quantum computing applications.

Moreover theoretical papers indicate 171-Yb as a very suitable candidate for long-range quantum communication, thanks to its telecom wavelength transition  $3P_0 \leftrightarrow 3D_1$  at 1389 nm [Y. Li et al., arXiv:2401.04075]. At this wavelength optical fibers have lower losses compared to the visible range, allowing long range propagation.

The apparatus shall be made of two distinct sections: a two stage cooling section and a science chamber equipped with an optical cavity. In the first section Yb atoms emitted by a hot source are collected and cooled to temperatures of a few  $\mu\text{K}$ , by means of magneto optical trapping (MOT) in two and three dimensions. These atoms are then transferred to the science chamber via a travelling wave optical lattice. Once in the science chamber, they are stored in an optical dipole trap (ODT) where they are further cooled and prepared to be used in experimental sequences.



First year: during the first year the focus will be on finalizing the design of the ultra-high vacuum apparatus, and the optical cavity assembly. Assembling the vacuum apparatus regarding the cooling stage and realizing the 2D- and 3D-MOT.

Second year: during the second year, the science chamber section, including the optical cavity, will be realized and tested and will be integrated in the already built vacuum setup. The travelling-wave optical lattice will be realized.

Third year: the loading of Yb atoms into the ODT reservoir and subsequently in the optical tweezers will be perfected and the atom cavity interaction will be studied.

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Supervisor 1: *Matteo Marinelli*

Supervisor 2: *Francesco Scazza*

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Low Temperature Physics: gases and Fluids	Pena Ardila	2	16
Modern tools for computational physics	Coslovich	1.5	12
Modern experiments in quantum optics and quantum information	Bruno, Scazza, Marinelli	1	8
Decoherence in open quantum systems	Carlesso	2	16
Non-equilibrium approaches to complex quantum materials	Fausti	1	8
Neural networks: a hands-on introduction	Goldt	1.5	12
		9	72





# **Development of Techniques and Applications for Scattering-Based X-Ray Imaging and Tomography**

**Giovanni Lemma**

*Traditional X-ray imaging provides only a projection of the attenuation introduced by the sample on incident radiation. In the past decades techniques have been developed to capture how the sample scatters X-rays, offering richer structural information. This PhD project aims to enhance existing data acquisition methods and extraction algorithms, possibly extending them to operate with partially coherent X-ray sources. As part of the PhD work, improving scattering-based X-ray imaging procedures will also serve as a starting point to combine these techniques with tomography, to produce a three-dimensional map of the orientation of micro- and nanostructures of the sample, with interesting medical and industrial applications.*

Information about the phase of the electromagnetic radiation, inaccessible to X-ray detectors, can be indirectly retrieved by analyzing the modulation of a structured illumination generated using membranes or random diffusers. This approach, known as modulation-based imaging, enables the extraction of phase information, including the amount of small-angle X-ray scattering, coined dark-field signal [1]. Creating a map of how each region of a sample scatters X-rays, i.e., the dark-field image, provides richer structural information when combined with the conventional attenuation data obtained in traditional X-ray imaging.

This PhD project, conducted within the framework of the S-BaXIT (Scattering-Based X-ray Imaging and Tomography) project, focuses on advancing these scattering-based imaging techniques. The work will be carried out mainly at the OptImaTo (Optimal Imaging and Tomography) Laboratory (Trieste, Italy), an X-ray laboratory tailored for phase-sensitive techniques [2]. Some synchrotron-based experiments are also planned, to complement the measurements made in the laboratory.

A major focus of this research is to enhance the acquisition procedures and algorithms used to extract scattering information from raw data. In particular, special attention will be given to reducing artefacts and spurious contributions to the dark-field signal that arise when using polychromatic X-ray sources. These improvements are instrumental in consolidating modulation-based imaging as a routine technique at OptImaTo, enabling higher-quality measurements and fostering collaborations with industrial and medical partners, which in turn will stimulate further development and refinement of the techniques through the increasing availability and diversity of samples.

Beyond refining existing methods, the project also aims to develop new, more robust and efficient algorithms, potentially by reformulating the problem in alternative domains (e.g., the wavelet domain).



Another key goal is to integrate scattering-based imaging with tomography to preserve directional scattering information. This integration will enable the implementation of tensor tomography, which reconstructs the main orientation of structural features within each voxel. While this approach is already established at synchrotron facilities, developing a laboratory-based implementation is a crucial step for OptImaTo. An example of tensor tomography previously performed within the S-BaXIT project [3] at PSI synchrotron (Villigen, Switzerland) is reported in Figure 1.

Finally, the project will explore the connection between dark-field signal and the reciprocal space characterization locally obtained with small-angle scattering techniques such as SAXS and USAXS. This effort will contribute to a deeper understanding of the microstructural information encoded in different scattering regimes.

#### References:

- [1]: Marie-Christine Zdora, *State of Art Speckle-Based Phase-Contrast and Dark-Field Imaging*, Journal of Imaging 2018, 4(5), 60.
- [2]: Vittorio Di Trapani et al., *Speckle-based imaging (SBI) applications with spectral photon counting detectors at the newly established OPTIMATO (OPTimal IMAGING and TOMography) laboratory*, Journal of Instrumentation 2024, 19, C01018.
- [3]: Ginevra Lautizi et al., *Robust dark-field signal extraction for modulation-based X-ray tensor tomography*, Applied Physics Letters, 125, 264103 (2024).

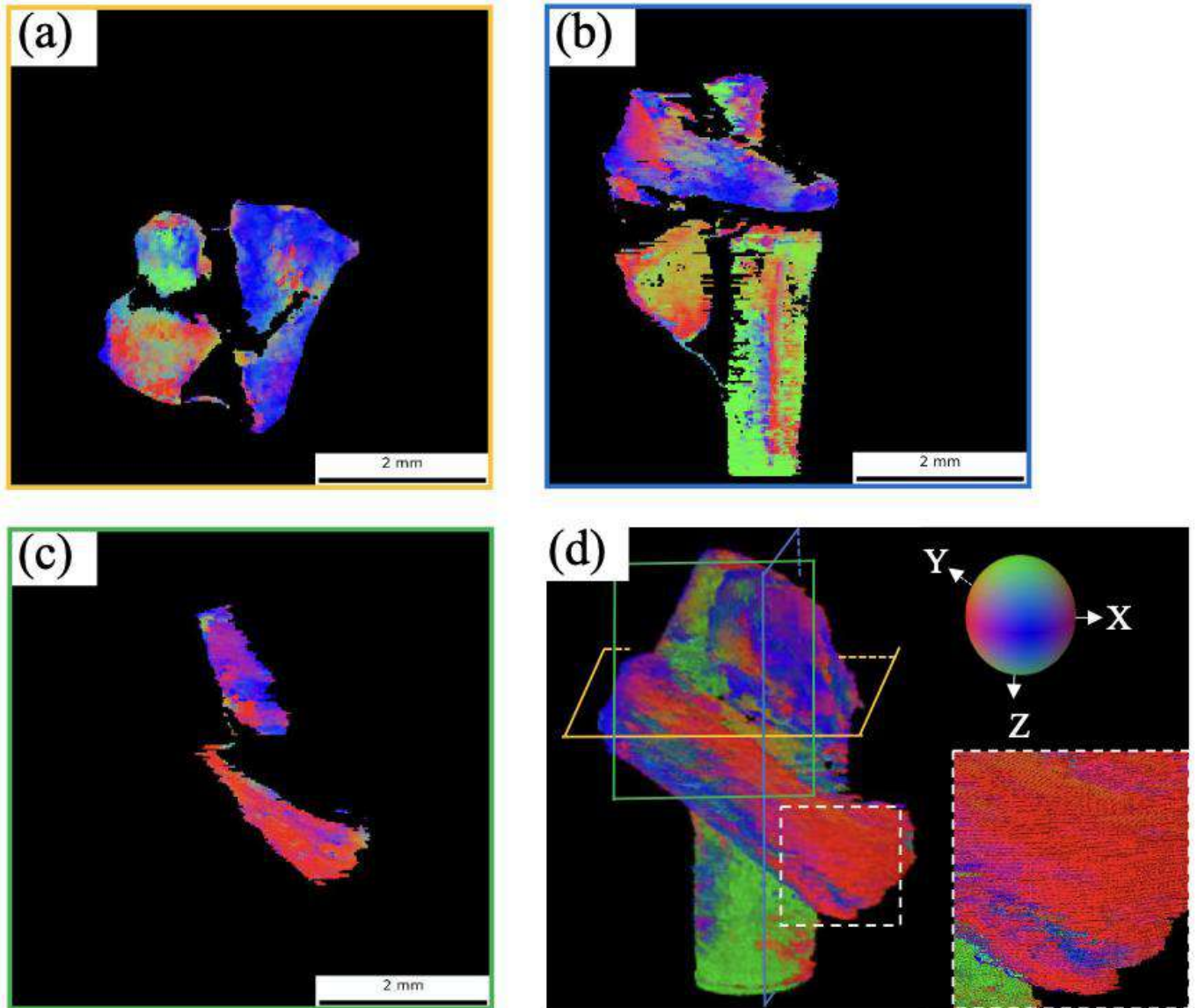


Figure 1: XTT results of a carbon fiber sample made using 4 unidirectional carbon fibers rods cut and glued in 4 different positions. (a) An axial slice, (b) a coronal slice and (c) a sagittal slice of the sample volume. The color is an RGB representation of the local structure orientation. The color ball is shown in (d) and it is symmetric with respect to the  $x$ - $y$ ,  $x$ - $z$ , and  $y$ - $z$  planes. (d) A 3D visualization of the reconstructed scattering tensor. In this representation, each arrow's orientation corresponds to the main direction in each voxel. The colorful planes indicate the slices shown in the other panels. The white inset shows a zoomed region to appreciate the directional information. The image is reproduced from [3].

Supervisor 1: *Pierre Thibault*

Supervisor 2: *Luca Brombal*



List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Advanced data analysis techniques with machine and deep learning	LUPARELLO	2	16
The physics of imaging with X-rays and associated X-ray detectors	MENK/ BROMBAL	3	24
Bayesian Statistics with Numerical Applications	MILOTTI	3	24
Numerical Methods for Inverse Problems (First year master degree (laurea magistrale) in mathematics, Università degli Studi di Trieste)	NOVATI	6 (4 of which will be recognized)	48
		8 from regular PhD teachings + 4 from a master teaching TOT: 12	64 from regular PhD teaching



# Charged Polarons in Low-Dimensional Ultracold Quantum Gases

Davit Mdinaradze

## SUMMARY

*This project will explore the ground-state and non equilibrium properties of ions immersed in a low dimensional ultracold quantum gases. In lower dimension quantum fluctuations become significantly enhanced, altering the polaron formation, and effective interactions between charged quasiparticles. A powerful combination of theoretical insight and cutting-edge computational tools will be used to tackle the project, with quantum Monte Carlo methods playing a central role. The results will be relevant for quantum technologies, such as buffer-gas-cooled ion qubits [1] and analog quantum simulators based on low-dimensional ion crystals [2].*

Recent progress in ultracold atom–ion experiments has opened a promising route toward studying strongly correlated quantum impurities. Because atom–ion interactions are long-ranged, ionic polarons display qualitatively richer behavior than their neutral counterparts. Whereas most of the theoretical and experimental work up to now has focused on three-dimensional systems, we discuss reduced-dimensional setups, where quantum fluctuations have a dramatically enhanced role and are expected to give rise to markedly different physics. The PhD project is split in three main objectives:

### **Quantum fluctuations and bipolaron formation.**

In lower dimensions, the enhanced quantum fluctuations dramatically change the ground-state properties of ionic polarons and can strongly affect the stability of bipolarons (bound states of two polarons). We focus on investigating the role of the dimensionality on the formation of the mesoscopic many-body bound states and probe, whether polarons can amplify nonlinear effects originating from inherent quantum fluctuations, unlike the situation in higher-dimensional systems. In addition, the dimensionality reduction suppresses the three-body inelastic process undesirable in experiments.

### **Quantum gates and buffer-gas cooling**

A very promising application of low-dimensional ionic polarons arises in trapped-ion quantum information processing. We will focus on the effect of buffer-gas cooling in low-dimensional atomic environments on motional heating and, consequently, on gate fidelities between ion qubits. While in three-dimensional geometries motional decoherence due to atom-ion collisions sets considerable limits to performance [1], the reduction of dimensionality alters the structure of available scattering channels and may reduce these harmful effects. Within a master-equation approach, we will quantify whether reduced-dimensionality trapped-ion platforms cooled by a buffer gas can potentially outperform conventional laser-cooled architectures.



## Quantum simulation with 1D/2D ion crystals

A hybrid quantum-simulation platform will be developed, in which a low-dimensional ion crystal will be coupled to fermionic atoms to simulate electrons in the lattice [2] or with bosons if one is interested in the coupling with phonons. This will enable the study of paradigmatic many-body phenomena, such as Peierls transition or Fröhlich-type electron-phonon coupling, in a completely controllable environment. The goal is to study how the tuning of atom-ion interactions and geometry affects the distribution of long-range correlations and the emergence of quantum fluctuations in strongly correlated ground states.

### Methods.

The project will mainly use Quantum Monte Carlo simulations, such as variational Monte Carlo and diffusion Monte Carlo, for accessing ground-state properties in strongly interacting regimes beyond perturbative methods. These numerical techniques will be combined with semi-analytical methods, such as coherent variational ansätze and master-equation methods, for example; on spin-boson models, as well as time-dependent Gross-Pitaevskii equations to investigate the dynamical behavior of the system.

These combined objectives and methodologies will provide new insights into the impurity physics of quantum many-body systems and will advance the quest for the experimental realization and control of ionic polarons in ultracold atom-ion platforms, a research area still in its infancy. The results will find direct applications in emerging quantum technologies.

[1] *Phonon-mediated quantum gates in trapped ions coupled to an ultracold atomic gas* L. Oghittu, A. Safavi-Naini, A. Negretti, and R. Gerritsma

[2] *Emulating Solid-State Physics with a Hybrid System of Ultracold Ions and Atoms* U. Bissbort, D. Cocks, A. Negretti, Z. Idziaszek, T. Calarco, F. Schmidt-Kaler, W. Hofstetter, and R. Gerritsma

---

Supervisor: Luis Aldemar Peña Ardila  
Cosupervisor: *Federico Becca*





List of courses to be taken (pending confirmation)

Title	Professor	CFU	Hours
Many-Body Simulations. Monte Carlo	F. Becca	3	24
Many-Body Simulations. Exact and Renormalization methods (SISSA)	M. Collura	3	24
Low Temperature Physics: gases and Fluids	L. Ardila	2	16
		8	64



# **Measurement of Helium-3 and Helium-4 production with the ALICE experiment**

**Cristian Moscatelli**

## **SUMMARY**

The study of light (anti)nuclei production mechanisms is a key objective in nuclear physics, and offers a unique opportunity to probe physics beyond the Standard Model. During my PhD, I will investigate (anti)<sup>3</sup>He and (anti)<sup>4</sup>He production in pp collisions at the Large Hadron Collider. The project combines both phenomenological and experimental aspects. I will enhance current simulation tools to more accurately reproduce experimental observations, and perform the first measurement of (anti)<sup>3</sup>He and (anti)<sup>4</sup>He production. The comparison between simulations and experimental results could provide new insights into the mechanisms governing light (anti)nuclei production, helping to interpret any future antinuclei detection in space.

## **Project description**

My PhD project is conducted in collaboration with the ALICE experiment and focuses on the production of light (anti)nuclei in proton-proton collisions during Run 3 at the Large Hadron Collider (LHC). This work extends the research I started in my Master's thesis.

The production of light (anti)nuclei is of central importance for testing physics beyond the Standard Model. In our Universe, there are few known sources of light antinuclei. Standard sources include high-energy interactions between cosmic rays and the interstellar medium, while more exotic scenarios suggest that light antinuclei could originate from the annihilation or decay of dark matter [1]. A few tentative antinuclei candidates have been observed by space experiments, renewing the interest in studying their formation mechanisms, as they could serve as a probe for new physics [2].

On Earth, the only precise way to study (anti)nuclei formation mechanisms is through high-energy collisions at particles accelerators. These studies help constrain models of light antinuclei production in cosmic-ray–interstellar-medium interactions, which are analogous to proton-proton collisions at accelerators. Such investigations are therefore crucial for interpreting future measurements of cosmic antinuclei.

The LHC is the World's most powerful particle accelerator, and the ALICE detector, with its excellent particle tracking and identification capabilities, is suited to study light (anti)nuclei yields [3]. The production and interaction of light (anti)nuclei are currently under intense debate. Two phenomenological approaches have been shown to describe their formation in hadronic collisions: statistical hadronization models [4] and coalescence models [5].

My PhD project combines both phenomenological and experimental aspects. On the phenomenological side, the first objective is to improve the simulation of (anti)<sup>3</sup>He production in the PYTHIA 8 event generator [6], which enables to simulate high-energy hadronic collisions. In my



Master's thesis, I implemented  $(\text{anti})^3\text{He}$  production in PYTHIA 8 using a simple coalescence model through the reaction  $p + d \rightarrow ^3\text{He} + \pi^0$ .

The first part of my PhD program focuses on implementing new reaction channels, each with a cross section tuned to experimental observations.

I will also work on the implementation, for the first time, of  $(\text{anti})^4\text{He}$  production in PYTHIA 8 using a coalescence approach. In this case,  $(\text{anti})^4\text{He}$  can form via the coalescence of a  $(\text{anti})^3\text{He}$  and a  $(\text{anti})\text{neutron}$ , or of a  $(\text{anti})\text{tritium}$  and a  $(\text{anti})\text{proton}$ . The corresponding reaction cross sections will be obtained from experimental measurements.

On the experimental side, my analysis will begin by refining the measurement of the  $(\text{anti})^3\text{He}$  spectrum I performed in my Master's thesis. Specifically, I will evaluate systematic uncertainties and improve the Monte Carlo simulation used to estimate acceptance and efficiency corrections. The next step will be the first-ever measurement of  $(\text{anti})^3\text{He}$  production inside and outside jets (narrow sprays of collimated particles), identified using the anti- $k_T$  algorithm [7]. This analysis was previously unfeasible due to the limited statistics of Run 2, but Run 3 is expected to yield over 10 million  $(\text{anti})^3\text{He}$  candidates, enabling high-precision measurements. From these data, I will extract the coalescence parameter  $B_3$ , which quantifies the probability of  $(\text{anti})^3\text{He}$  formation. Theoretical models predict higher  $B_3$  values inside jets, due to the closer proximity of  $(\text{anti})\text{nucleons}$  in phase space.

Regarding  $(\text{anti})^4\text{He}$ , the primary goal is to measure its inclusive spectrum. During Run 3, around 150  $(\text{anti})^4\text{He}$  candidates were reconstructed in the TPC, enabling the first measurement of their production. The full Run 3 dataset will provide sufficient statistics to perform a precise inclusive measurement.

These results will support the validation of phenomenological models of nuclear coalescence, enhance our understanding of hadronization processes involving multi-baryon system, and contribute to indirect searches for physics beyond the Standard Model.

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Supervisor 1: *Prof.ssa Valentina Zaccolo*  
Supervisor 2: *Prof.ssa Ramona Lea*  
Board group member: *Prof. Paolo Camerini*

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Quark Gluon Plasma: theory and experimental observations	Prof. Fragiaco	2	16
Advanced data analysis techniques with machine and deep learning	Prof.ssa Luparello	2	16
Introduction to RooFit	Prof. Pinamonti	2	16
Introduction to parallel computing	Prof. Tornatore	3	24
		9	72



## QUBRICS: bright, high-redshift quasars for Cosmology

Romeo Pallikkara

### SUMMARY

*Quasars are very bright objects powered by accretion onto super-massive black holes. The absorption lines superimposed to the quasar continuum spectra by intervening clouds of cold dust help us study the intergalactic medium and the early universe. My project focuses on finding new and bright distant quasars in the southern sky using data from public surveys. Stars and galaxies can look very similar to quasars, especially the faint ones, so we will use statistical and machine-learning methods to detect quasars more reliably. We also aim to measure their redshifts more accurately and build a comprehensive catalogue. This work will improve our understanding of quasar evolution, demography and help identify the best targets for future observations.*

Quasi-stellar objects (also known as QSOs or quasars) are extremely bright extra-galactic sources powered by a supermassive black hole at the center of their host galaxies. These distant objects act as cosmic beacons to study the early universe and the intervening medium between the QSO and the observer. Through QSO absorption lines it is possible to study the physical conditions of the primordial universe, large-scale structure formation, provide constraints on cosmological parameters, and understanding the recombination phase of the universe.

The QUBRICS (QUasars as BRight beacons for Cosmology in the Southern hemisphere; Calderone et al., 2019) project aims to identify new, bright, high-redshift ( $z > 2.5$ ) QSOs in the Southern Hemisphere, which has historically been underrepresented due to the bias in past large-scale surveys. The project exploits photometric data from publicly available surveys, analyzed using machine-learning methods, to identify QSO candidates that can be observed spectroscopically using facilities in the South.

Identifying these high- $z$  objects is challenging, as contaminating sources like stars and galaxies are orders of magnitude more numerous than QSOs, especially the bright ones. Use of probabilistic classification models, including Probabilistic Random Forests, eXtreme Gradient Boosting, and other deep-learning frameworks, will be carried out to enhance the precision and accuracy of quasar selection. Another challenge is calculating the redshift of these identified sources accurately and determining the completeness of the sample. We plan to address this by exploring and deploying Gaussian Processes, StratLearn, and other Bayesian approaches for refining redshift prediction models. We also plan to develop



multi-objective optimization heuristics that balance dataset completeness with the minimization of unnecessary spectroscopic follow-ups.

In seven years, QUBRICS has been able to identify more than 1,000 new QSOs, and the database is continuously being updated. The QSO luminosity function helps us understand the distribution of QSO luminosities and AGN activity. During my PhD, we also plan to look into several key challenges: improving the success rate of identifying new QSOs at fainter magnitudes, increasing the completeness of our samples at  $z > 5.2$ , and obtaining tighter constraints on the luminosity function around  $z \sim 5.5$ . This particular redshift range is challenging due to the tendency of models to misclassify M-dwarf stars as QSOs. We also aim to identify the most promising candidates for future redshift-drift (Sandage test) observations.

By the end of my PhD, we expect to develop an improved QSO selection pipeline with better performance at fainter magnitudes and at high redshifts. We also aim to achieve more accurate photometric redshift estimations using the probabilistic and Bayesian methods explored in the project. This work is expected to produce an updated and more complete QUBRICS high- $z$  QSO catalog with reduced contamination from stars, along with tighter constraints on the QSO luminosity function

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Supervisor 1: Giorgio Calderone  
Supervisor 2: Stefano Cristiani  
Co-supervisor: Marisa Girardi

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Active galactic nuclei	FIORE	1,5	12
Galaxy formation	DE LUCIA	1,5	12
Introduction to parallel computing	TORNATORE	3	24
Intergalactic Medium	Stefano Cristiani	1	8
Imaging with X-rays -fundamentals and applications	THIBAUT / DI TRAPANI	2	16
		9	72



# Understanding the Chemical Evolution of the Milky Way and Local Group dSph and dlrr galaxies

Emanuele Pepe

## SUMMARY

*This PhD project investigates how the Milky Way and its neighboring dwarf galaxies have evolved chemically over time. By modeling how different regions of the Milky Way formed and enriched themselves with elements from stars, we will explore how stellar nucleosynthesis, gas flows, and stellar migration shape the Galaxy stellar population. The study will then extend to nearby dwarf galaxies, examining how their interactions with the Milky Way, through gravity, gas exchange, and tidal forces, have influenced their evolution. Using modern observations and statistical methods, the project aims to reveal how internal processes and external interactions have shaped the chemical history of our local galaxies.*

In the study of the Milky Way (MW), we distinguish four main stellar populations, each characterized by distinct kinematics, chemical abundances, ages, and spatial distributions: the central bulge, the thick disk, the thin disk, and the stellar halo. This PhD project aims to perform a detailed modeling of the chemical evolution of these MW components in the light of the most recent spectroscopic surveys (APOGEE DR17; GALAH DR4) and more precise stellar ages estimates from asteroseismology and machine learning (Anders et al. 2023; Barbolato et al. 2025). We will also study dwarf irregular (dlrr) and dwarf spheroidal (dSph) galaxies in the Local Group, to reconstruct the role that their interaction with the MW has played in its overall evolution.

During the first year, we will investigate the evolution of the Galactic thick and thin disks using state-of-the-art chemical evolution models (Spitoni et al. 2019, 2020, 2024; Palla et al. 2020; Palla 2021; Pepe et al. 2025). These models will include gas inflow and outflow processes, as well as nucleosynthetic yields from low-, intermediate-, and high-mass stars. We will construct a multizone model of the MW disk that follows the chemical enrichment of multiple annular regions (2 kpc wide) centered at different Galactocentric radii (from 4 to 18 kpc). This framework will enable us to explore how different assumptions, such as stellar yields for massive binary stars (Farmer et al. 2023; Pepe et al. 2025; Ma et al. 2025), Type Ia supernova (SNe Ia) progenitor models, expressed through distinct delay-time distributions (Matteucci & Recchi 2001; Greggio 2005; Strolger et al. 2005; Mannucci et al. 2006; Totani et al. 2008), and the inclusion of stellar radial migration (Frankel et al. 2018; Palla et al. 2022; Spitoni et al. 2025), affect the chemical evolution of the MW thin and thick disks. The models will be constrained using data from recent large spectroscopic surveys such as APOGEE DR17 (Abdurro'uf et al. 2022) and GALAH DR 4 (Buder et al. 2025), complemented by asteroseismic constraints and the most recent analyses of RR Lyrae stars (D'Orazi et al. 2024; Bono et al. submitted to ApJ).





During the second year, we will develop an integrated model that simultaneously follows the evolution of all Galactic components, enabling us to investigate their mutual interactions and the resulting impact on the chemical evolution of multiple elements.

In the third year, we will extend this framework to model the detailed chemical evolution of selected dIrr and dSph galaxies, focusing on those currently or previously interacting with the MW. These models will be constrained using high-precision star formation histories (SFHs) derived from color–magnitude diagram (CMD) fitting, based on deep photometric observations. For instance, the Large Magellanic Cloud (LMC), the nearest and best-studied irregular galaxy, offers an ideal test case. Using data from the SMASH survey and CMD fitting techniques, we will map the chemical abundance patterns across different regions of the LMC and extend this analysis to the Small Magellanic Cloud (SMC), also considering the interactions indicated in Burhenne et al. (2025) and Lu et al. (2025). Among dwarf galaxies, particular attention will be given to Sagittarius, whose pericentric passages are thought to have influenced and triggered star formation activity in the solar neighborhood (Ruiz-Lara et al. 2020).

To robustly explore the parameter space of our chemical evolution models and quantify the uncertainties, we will adopt a Bayesian framework. Inference will be performed using advanced Markov Chain Monte Carlo (MCMC) techniques (Spitoni et al. 2020, 2021), allowing us to derive posterior probability distributions for key parameters such as star formation efficiency, infall timescales, and galactic wind strengths. A major goal of this project is to assess the influence of environmental effects, such as tidal interactions, ram pressure stripping, and gas accretion from the MW and other galaxies, on the chemical enrichment histories of its satellite systems. By comparing model predictions with observed abundance patterns and SFHs, this work aims to elucidate the interplay between internal evolutionary processes and external perturbations in shaping the chemical evolution of low-mass galaxies in the Local Group.

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Palla, M., Santos-Peral, P., Recio-Blanco, A., & Matteucci, F. 2022, *A&A*, 663, A125  
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Supervisor 1: Emanuele Spitoni

Supervisor 2: Maria Francesca Matteucci

Supervisor 3: Marisa Girardi

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Bayesian Statistics with Numerical Applications	Milotti	3	24
Active Galactic Nuclei	Fiore	1.5	12
Introduction to parallel computing	Tornatore	3	24
Galaxy formation	De Lucia	1.5	12
Galactic Archaeology in the era of large surveys. From chemical abundances to galaxy formation and evolution	Matteucci	1.5	12
		10.5	84



# Metal enrichment of the intergalactic medium and the nature of the first ionizing sources

Christian Piscitelli

## SUMMARY

*A few hundred million years after the Big Bang, the Universe was cold, dark, and filled with neutral hydrogen. The first stars and galaxies began to illuminate this environment, creating regions of ionized gas and releasing some of the heavy elements formed in their interiors. These elements were carried out of the early galaxies and mixed with the diffuse gas that fills the space between galaxies. By studying how this gas absorbs light in the spectra of distant quasars, we can measure the presence and amount of these heavy elements. This project aims to determine the level of chemical enrichment in the intergalactic gas using a new set of highly detailed quasar spectra at high redshift. The results will be compared with advanced numerical simulations to assess how many heavy elements are present, how they are distributed, and what they can reveal about the properties of the first luminous sources in the Universe.*

A few hundred million years after the Big Bang, the Universe was a cold and dark place, filled with neutral hydrogen (Fan et al. 2006). The first stars and galaxies that formed began to carve out ionized bubbles around them through the emission of photons with energies greater than 13.6 eV. At the same time, these early sources expelled some of the metals produced in stellar interiors, enriching the surrounding medium (Stark 2016). This marked the beginning of the so-called Cosmic Reionization, considered the last major phase transition in the history of the Universe (Dayal and Ferrara, 2018; Davies F.B., 2018).

The heavy elements released during this early epoch are expected to be found in the low-density gas near the cosmic mean density, known as the intergalactic medium (IGM), the material that fills the space between galaxies.

This material preserves the imprint of the earliest enrichment events with minimal disturbance from later galaxy interactions, acting as a fossil record of the first billion years. By comparing the observed abundance and distribution of metals in the IGM with theoretical predictions, it becomes possible to infer key properties of the first ionizing sources, which are thought to include both early galaxies and the first active galactic nuclei, with luminous quasars contributing significantly.

In particular, the latter represent exceptionally powerful torches, illuminating the intervening cosmic web and enabling the detection of even extremely weak absorption lines. In some



cases, they can also produce high-velocity outflows extending hundreds of parsecs, capable of influencing and ionizing their surroundings.

Despite their importance, only a limited number of quasar spectra currently have sufficient spectral resolution and signal-to-noise ratio to allow precise measurements of the metal content in the IGM.

In order to determine the metallicity of the IGM, in my PhD project I plan to analyze a statistical sample of new, very high-resolution and high signal-to-noise quasar spectra in the redshift range  $z \sim 3.5\text{--}4.5$ , through high-quality spectroscopic data from ESPRESSO spectrograph (Pepe et al. 2021), mounted on the Very Large Telescope (VLT), which is able to reach a spectral resolution of  $R \sim 100.000$  for each quasar spectrum, making it possible to resolve blended absorption lines, detect weak features, and examine the detailed velocity structure of the absorbing gas. Such precision is essential for distinguishing between different phases of the IGM and for identifying signatures of early metal enrichment.

The first and the second year will be dedicated to the application of both direct line detection methods and statistical techniques designed to measure the cumulative metal content of the IGM.

During the third year, these observational results will be compared with predictions from state-of-the-art simulations and semi-analytical models.

Finally, the ultimate goals of the project are to assess the presence of metals in the IGM, quantify their abundance, evaluate their contribution to the total metal budget at high-redshift, and, through comparison with simulations, infer the general properties of the first ionizing sources, describing how these sources can ionize the IGM.

The project is funded by the ERC Synergy Grant “RECAP”. Being a part of this Synergy Grant, it will be possible to work within an international collaboration, with opportunities for frequent visits to partner institutions and extensive interaction with a large group of researchers working together to answer fundamental questions about the epoch of Reionization.

#### Reference:

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“The Opacity of the Intergalactic Medium Measured along Quasar Sightlines at  $z \sim 6$ ”, Eilers Anna-Christina, et al. 2018, *ApJ* 864.1, 53, p. 53.

“Outflows and the Physical Properties of Quasars”, Ganguly, R. et al. 2007, *ApJ* 665.2, pp. 990–1003.

“Reionization of the Intergalactic Medium and the Damping Wing of the Gunn-Peterson Trough”, Miralda-Escudé, J., July 2018, *ApJ* 501.1, pp. 15–22.

“The Lyman Alpha Forest in the Spectra of QSOs”, Rauch, Michael et al. 1998, *Annu. Rev. Astron. Astrophys.* 36, pp. 267–316.

“Nuclear Winds Drive Large-Scale Cold Gas Outflows in Quasars during the Reionization Epoch”, Zhu, Y. et al. 2025, *Arxiv* e-prints.

“ESPRESSO at VLT. On-sky performance and first results”, Pepe, F. et al. 2021, *A&A*, 645, A96.

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Supervisor Scientifico: *Valentina d’Odorico*  
Supervisor di Collegio: *Stefano Borgani*

Title	Teacher	CFU	Hours
Active Galactic Nuclei	FIORE	1,5	12
Galaxy Formation	DE LUCIA	1,5	12
Galactic Archaeology in the era of large surveys. From chemical abundances to galaxy formation and evolution	MATTEUCCI	1,5	12
Advanced data analysis techniques with machine and deep learning	LUPARELLO	2	16
Formation of cosmic structures	BORGANI	3	24
		9.5	76



# Theory and Modelling of X-ray Chiral Spectroscopies

## Manuel Fernando Sánchez Alarcón

### SUMMARY

*This project explores how molecules that come in left- and right-handed forms interact differently with X-ray light. It develops two complementary theoretical approaches. The first models how molecules respond when illuminated with X-ray beams that carry a twisted wavefront, which probes the local motion of electrons beyond the usual approximations. The second extends an existing real-time method to simulate how electrons move when exposed to circularly polarized X-rays, allowing these differences in response to be predicted from the time evolution of the system. Both approaches will be applied to realistic environments, including liquids. Together, they aim to clarify what structural information about chiral molecules can be extracted from advanced X-ray measurements.*

### PROJECT DESCRIPTION:

Chiral molecules exist in two non-superimposable mirror-image forms whose distinct response to light makes chiroptical spectroscopies valuable tools for structural characterization. Extending these techniques to the X-ray regime enables access to element-specific core-level excitations and local electronic asymmetries. This project aims to model X-ray chiral responses using two approaches, each suited to a different class of measurements: X-ray helical dichroism (HD) and X-ray circular dichroism (CD).

A first direction is motivated by the experimental demonstration of hard X-ray helical dichroism (HD) by Rouxel et al. [1]. HD measures the differential absorption between vortex beams with opposite orbital angular momentum. The observable reflects the interaction between the spatial phase structure of the beam and the transition current densities involved in core-level excitations, requiring a theoretical description beyond the dipole approximation. The results reported by Rouxel et al. show measurable HD signals in powder samples, indicating that X-ray chiral responses can be accessed in orientationally disordered media.

A second, independent direction builds on the real-time propagation framework for electronic CD introduced Coccia and collaborators [2]. This method propagates the time-dependent Schrödinger equation in the basis of field-free electronic eigenstates, allowing CD spectra to be computed by directly accessing the photoinduced electron dynamics. The approach reproduces linear-response results and matches available experimental data for several test molecules. Its formulation grants access to the time-domain evolution of the wavefunction and the dependence of chiral signals on electronic-state populations. In this project, the real-time electronic CD method will be extended to compute X-ray CD spectra.

The PhD work will therefore incorporate two distinct modelling strategies; each applied in the experimental conditions for which it is best suited. Both will be used to investigate chiral responses in realistic environments, including liquid samples, where orientational averaging and solvent effects play a significant role. Together, these modelling tools will support the interpretation of future X-ray chiral measurements and contribute to clarifying the structural information accessible through HD and CD in non-crystalline media.



## References:

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- 

Supervisor 1: *Majed Chergui*

Supervisor 2: *Emanuele Coccia*

Supervisor 3: *Claudio Masciovecchio*

Supervisor 4: *Pierre Thibault*

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Advanced Data Analysis Techniques with Machine and Deep Learning	Luparello	2	16
Imaging with X-rays: Fundamentals and Applications	Thibault and Di Trappani	2	16 (8+8)
Free Electron Laser and Synchrotron Based Spectroscopies: Getting to the Nanometer with Femtosecond Resolution	Masciovecchio	2.5	20
Introduction to Density Functional Theory	Peressi/Bidoggia	2	16 (8+8)
Modern Tools for Computational Physics	Coslovich	1.5	12
		10	80





# Axions in the Early Universe

## RAFFAELE TIEDE

### SUMMARY

*The aim of this PhD is to explore some possible light Dark Matter models, in particular involving pseudo-Goldstone bosons (axions, axion-like particles). Of the possible scenarios we consider:*

- **(Kinetic) Misalignment:** *oscillations in a classical field describe the Dark Matter abundance; we study the mechanism also on a lattice.*
- **Axion-portal models:** *the particle acts as a bridge between a secluded Dark Sector and the Standard Model fields.*

Axion models are both theoretically compelling and phenomenologically rich. Originally introduced as a natural solution to the strong CP problem, axions and axion-like particles (ALPs) also provide exceptionally well-motivated candidates for the dark matter of the Universe. Their cosmological dynamics—such as the formation of strings and domain walls—can leave observable imprints on the cosmic microwave background, the matter power spectrum, and the stochastic gravitational-wave background. Moreover, axions arise abundantly in UV-complete theories such as string compactifications, where entire axion “landscapes” or “axiverses” are a generic outcome.

Axion dark matter can be produced through several complementary mechanisms (parametric resonance, (kinetic) misalignment, interactions), making the scenario robust against assumptions about the early Universe.

In QFT, once a UV continuous symmetry is spontaneously broken by a scalar potential taking a VEV, the complex scalar can be decomposed into two modes: one is a heavy massive mode which is usually integrated out in the effective theory, and the other is the pseudo-Goldstone boson (a naturally light field describing the angular dependence of the UV scalar field, usually referred to as axion-like particle). It can happen that at the lowest energy point of the radial mode, a non-flat potential develops (e.g. QCD phase transition for the axion), generating a small mass for the field.

The initial condition of the field does usually not correspond to the minimum of this angular potential, and the field starts oscillating inside the minimum. The energy density of these oscillations redshifts exactly like matter, making this an interesting and plausible dark matter candidate. The magnitude of the energy density depends on the initial condition, the time of the symmetry breaking and the amplitude of this potential.

This model comes with tuning issues if we want the axion to describe the entire dark matter budget, but can be solved by giving an initial angular velocity to the UV field through a higher order term in the Lagrangian, which explicitly breaks the UV symmetry. The breaking occurs at high energy scales, generating a torque on the field, making it rotate.



In order to appreciate these higher order terms, the radial mode must thus have a large initial value.

Two interesting mechanisms which are able to generate this initial condition are:

- Hubble-scale negative mass squared drives the radial field to acquire a large temporary displacement from its true vacuum.
- de Sitter fluctuations during inflation push the initial value of the radial mode of the field to be much larger than the value at the minimum.

When the radial field relaxes, energy is transferred to angular modes of the pNGB.

Remarkably the initial angular kinetic energy effectively delays the onset of the oscillations (with respect to a field starting still), allowing for later spontaneous breakings (lower symmetry breaking scales, easier to access experimentally), without incurring into fine-tuning.

By solving the equations of motion on a Lattice it is possible to easily track the dynamics of the field with minimal effort, to get precise results for many different variations of the underlying model.

In this first model the DM is an oscillation in a classical field. Another more straight forward approach is to have DM be particle in nature.

A particularly interesting scenario is to have the axion-like particle be a portal connecting a dark sector (e.g. a light DM fermion motivated by chiral symmetry) to the standard model fields. Its dynamic can have effects on the evolution of the early universe (BBN, CMB, structures), and manifest through astrophysical signals today (Galactic centre 511 keV gamma-ray line).

These types of models are rich in phenomenology, and can solve multiple open problems at once, therefore they are strongly motivated. They can be tested by observing their effects on both BBN and CMB, the two most powerful observables of the early universe.

With the upcoming experiments improving sensitivities and broadening the testable parameter space, it is important to develop these types of flexible theories which can support a network of possible production mechanisms while providing elegant and natural solutions to multiple dark spots in the well-established theories.

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Supervisor 1: *Enrico Morgante*

Supervisor 2: *Roberto Valandro*

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
<b>Bayesian Statistics with Numerical Applications</b>	Edoardo Milotti	3	24



<b>Formation of cosmic structures</b>	Stefano Borgani Matteo Costanzi	3	24
<b>Beyond the Standard Model in the Early Universe (SISSA)</b>	Takeshi Kobayashi	4	32
		10	80



## A versatile instrument for X and gamma observations of the Universe and planetary surfaces

Tommaso Fagotto

### SUMMARY

*During this PhD project, I will work in the context of three CubeSat missions, all linked by an X-ray and gamma-ray spectrometer: SpIRIT, dedicated to the observation of Gamma Ray Bursts, TASTE, aiming to study the origin of Deimos, and PROGRex, focused on resource prospecting on the Moon. I will perform data analysis for SpIRIT, and conduct laboratory and X-ray fluorescence tests, as well as calibration activities, for TASTE and PROGRex, gaining experience in high-energy astrophysics, detector characterization and numerical modelling within international mission teams.*

CubeSats are small modular satellites, with a standard dimension of 10x10x10 cm<sup>3</sup> (1U), that use commercial off-the-shelf components for their electronics and structure.

This PhD project revolves around three CubeSat missions, all of which have in common an X-ray and gamma-ray spectrometer, designed, developed, integrated and tested by various INAF teams.

These three missions are:

- SpIRIT (Space Industry – Responsive – Intelligent – Thermal)
- ASI TASTE (Terrain Analyzer and Sample Tester Explorer)
- INAF PRORIS PROGRex (PROspecting the Moon with Gamma-Rays & X-rays)

SpIRIT is an Australia-Italy mission supported in Australia by the Australian Space Agency, operating since December 2023. The spectrometer hosted is used to probe the temporal emission of bright high-energy transients such as Gamma Ray Bursts.

TASTE is composed by a 9U orbiter and a 3U lander. Its objective is to study Deimos, one of the two Martian moons, to determine its origin. The spectrometer will measure the abundances of Calcium, Titanium, Iron, Thorium, Potassium and Uranium. The mission is currently in phase B, which is ending in September 2026, and it may be launched by the end of the decade.

PRORIS PROGRex goal is to develop a payload to be used on the surface of the Moon, on board of a rover, for resource prospecting. The X-ray spectrometer, along with an X-ray source, will perform X-ray Fluorescence (XRF) spectroscopy and assess the presence of Rare Earths, Titanium and Platinum Group Elements, in Thorium rich terrains. The project started on March 2025.

This project will involve researching on different topics for these missions. In particular:

- For SpIRIT, I'll conduct data analysis to observe light curves at different energy ranges, and I will also study the degradation of the spectrometer due to radiation damage
- For TASTE, I'll do laboratory tests to assess instrument performances, functional tests and calibration of the breadboard, including SDD and ASIC



• For PRORIS PROGRex, similarly to TASTE, I'll perform laboratory tests and calibration of the breadboard, with the addition of a demonstration model. Furthermore, I will conduct XRF tests aimed at optimizing the instrumentation and its use and at obtaining a calibration between emission lines and element abundances. For example, I need to understand the optimal distance between the X-ray source, the sensor and the sample, in order to arrange source and sensor inside the instrument and determine how to position the instrument in respect to the sample. These tests will first be performed with commercial sensors and X-ray sources, and then with a demonstrator in a chamber simulating the lunar environment (a thermal vacuum chamber with regolith, and an electron, proton and ion cannon that simulates cosmic rays). This will be an innovative study to see if vacuum, regolith or energetic particles affect fluorescence lines' emissivity. I'll then have to develop numerical models to compare the laboratory results. This will be research of technological scope and I will be involved first and foremost with the INAF-OATs team, but I'll also collaborate with the INAF teams of Bologna, Roma, Firenze and Napoli, and FBK. This project will let me gain experience in data analysis, related to high energy astrophysics, laboratory work on detectors and numerical modelling, but I will also have the opportunity to work actively on a space mission within a team, a valuable experience for possible future collaborations.

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Supervisor 1: *Fabrizio Fiore*

Supervisor 2: *Francesco Longo*

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Cosmic-Ray and Gamma-ray Astrophysics	MUNINI/ LONGO F	2	16 (10+6)
Advanced data analysis techniques with machine and deep learning	LUPARELLO	2	16
Astrophysical sources of gravitational waves	PRINCIPE	1,5	12
Gamma Ray Bursts: observations and theoretical implications	LONGO F	1,5	12
Introduction to parallel computing	TORNATORE	3	24
		10	80



# QUANTUM IMPURITIES UNDER THE MICROSCOPE

Antonino Vardè

## SUMMARY

*The focus of this PhD project is to perform quantum simulation experiments of fermionic many-body systems using ultracold fermionic ytterbium atoms. We will realize a state-of-the-art experimental setup, featuring single-atom control and detection to allow precise engineering and probing of strongly interacting regimes, which are challenging to simulate numerically. Atoms excited to a metastable electronic state will be employed to emulate the presence of impurities in a fermionic bath. Specifically, we aim to investigate the non-equilibrium dynamics of Fermi polarons and the celebrated Kondo model in reduced dimensionalities.*

A quantum simulator is a device in which a quantum mechanical system is engineered to have an effective Hamiltonian equivalent to that of the system one aims to simulate. One way to realize such a machine is by using ultracold neutral atoms, which enable the study of many-body quantum systems with unprecedented clarity and control[2]. In these platforms, atoms are cooled and confined exploiting light–atom interactions, and can be microscopically manipulated with the help of high-resolution optical techniques[1].

The main goal of this PhD project is the realization of such an apparatus, based on ultracold ytterbium atoms[3][4], to engineer fermionic many-body systems with a focus on studying the nonequilibrium dynamics of impurity-based models, such as Kondo Hamiltonians[5]. The key idea is to use fermionic isotopes in their electronic  $^1S_0$  ground state trapped in an optical dipole trap to obtain a degenerate Fermi gas, and atoms in the metastable  $^3P_0$  state, confined in optical tweezers, as individually controlled impurities, bringing them in mutual interaction[5].

### Project timeline during the three years of the PhD:

The first objective for the initial year is to cool a cloud of  $^{173}\text{Yb}$  atoms in an optical tweezer and/or an optical dipole trap to reach deep Fermi degeneracy. Additional activities will focus on implementing the 578 nm laser excitation to excite ytterbium atoms to the metastable  $^3P_0$  state along the ultranarrow clock transition, which will also provide an ultra-precise spectroscopic probe of many-body effects. In parallel, we will develop a spin-selective single-atom imaging technique based on the optical Stern–Gerlach effect[7].

The second year will begin with the implementation of optical tweezer traps at 759 nm, corresponding to the magic wavelength for the  $^1S_0 \rightarrow ^3P_0$  transition. These traps will be generated using holographic techniques, which will allow us to tune not only the size but



also, if needed, the shape of the trapping potential. A major development will focus on the capability to image atoms in a 2D gas individually in free space, namely the realization of a *Continuum Quantum Gas Microscope*[6]. This will dramatically increase the amount of information gained on the system's wavefunction in each experimental shot.

The third year will be dedicated to studying the interaction between the fermionic bath, composed by atoms in the  $^1S_0$  state, and one single or multiple impurities in the  $^3P_0$  state. A possible initial configuration involves creating a degenerate Fermi gas of  $^{173}\text{Yb}$  atoms and, in its vicinity, preparing single atoms excited to the  $^3P_0$  state. We will then overlap the two ensembles, quench the mutual interactions, and use the developed imaging tools to extract relevant information needed to characterize the evolution of the many-particle wavefunction. These experiments will be guided by the goal of gaining insight into the rich nonequilibrium physics of fermionic systems perturbed by mobile or localized impurities[5][8].

- [1] Barredo, Daniel; et al. (2018). "Synthetic three-dimensional atomic structures assembled atom by atom". *Nature* 561, pages 79–82.
- [2] Gross, Christian; Bloch, Immanuel (September 8, 2017). "Quantum simulations with ultracold atoms in optical lattices". *Nature*. 357 (6355): 995–1001.
- [3] O. Abdel Karim et al., Single-atom imaging of  $^{173}\text{Yb}$  in optical tweezers loaded by a five-beam magneto-optical trap, *Quantum Sci. Technol.* 10 045019 (2025)
- [4] A. Muzi Falconi et al., Microsecond-scale high-survival and number-resolved detection of ytterbium atom arrays, *arXiv:2507.01011* (2025)
- [5] Amaricci, Adriano; et al. (2025). "Engineering the Kondo impurity problem with alkaline-earth atom arrays". *arXiv:2505.14630*.
- [6] Joris Verstraten et al., In-situ Imaging of a Single-Atom Wave Packet in Continuous, 10.1103/PhysRevLett.134.083403
- [7] Shintaro Taie et al., Realization of  $SU(2)\times SU(6)$  Fermi System, *arXiv:1005.3670*
- [8] Pietro Massignan et al., Polarons, Dressed Molecules, and Itinerant Ferromagnetism in ultracold Fermi gases, *arXiv:1309.0219*





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Supervisor 1: *Francesco Scazza*

Supervisor 2: *Matteo Marinelli*

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Low Temperature Physics: Gases and Fluids	Pena Ardila	2	16
Modern Tools for Computational Physics	Coslovich	1.5	12
Modern Experiments in Quantum Optics and Quantum Information	Scazza/Marinelli	1	8
Decoherence in Open Quantum Systems	Carlesso	2	16
Neural Networks: A Hands-On Introduction	Goldt	1.5	12
Academic English		4	32
Public Speaking		1	8
From business model to business plan		1	8
		15.5	124



# Development of ultra-low material budget MAPS detectors for future physics experiments

Giovanni Vecil

## SUMMARY

*The investigation of the Quark-Gluon Plasma (QGP) produced by ultra-relativistic heavy-ion collisions strongly depends on the ability of tracking low-momentum and short-lived particles, which requires the construction of ultra-low material budget trackers. This project focuses on the development of silicon Monolithic Active Pixel Sensors (MAPS) and encompasses the laboratory characterisation of sensor prototypes, their integration in the detector units, and the simulation of the detector performance.*

The use of cutting-edge detector technologies in High Energy Physics is driving major progress in our understanding of Quantum Chromodynamics. In particular, the investigation on the *Quark-Gluon Plasma* (QGP) produced in ultra-relativistic heavy-ion collisions is the main physics objective of the ALICE experiment at the LHC at CERN. The analysis of the physical probes of QGP has greatly benefited from the adoption of Monolithic Active Pixel Sensors (MAPS) for the upgrade of the Inner Tracking System (ITS) in 2021. Consequently, strong interest has been demonstrated in the development of the future MAPS detectors dedicated to the study of QGP, such as the next upgrade of the ITS of the ALICE experiment (ITS3), the Silicon Vertex Tracker (SVT) of the ePIC experiment at the EIC at BNL, and the future ALICE 3 experiment at the LHC.

The project therefore focuses on the development of silicon MAPS for the construction of very low material budget trackers that can be placed as close as possible to the beam, thereby achieving optimal performance in the reconstruction of interaction and decay vertices and in the tracking of low-transverse momentum particles emerging from QGP. In this context, the project encompasses both the integration and characterisation of the detector units, as well as the data analysis and simulation needed to assess the performance improvements.

As part of the characterisation campaign of MAPS sensor prototypes for the ALICE ITS3 detector, I will study the energy response through the measurement of the signal *Time-over-Threshold* (ToT) for different particle energy depositions and different particle species. The main objective is to gain valuable knowledge of the analogue response of the sensors. However, this work also provides an opportunity to explore potential applications of MAPS technology in the construction of low-material budget and low-power consumption detectors for dosimetry and beam monitoring in hadron therapy, where energy loss measurements are performed to identify different particle species.



With the production of the final ITS3 sensor scheduled for spring 2026, I will focus on the full characterisation of its performance, for instance in terms of the impact of electronic noise, detection efficiency, and tracking resolution, through both laboratory and particle beam studies. At the same time, a careful optimisation and choice of operational parameters will be performed in preparation for its integration into the detector, planned for 2027–2028.

The construction of the ITS3 aims to improve the detector performance in the measurement of observables relevant to the study of QGP, such as the production of hadrons containing heavy quarks, where the ability to reconstruct the decay vertices of such short-lived particles is strongly dependent on the characteristics of the ITS. In this context, I will carry out simulations of the ITS3 performance and analyse the data collected by the ITS2, to assess the improvements brought by the introduction of innovative solutions in the detector layout and by the reduced material budget (from 0.36%  $X_0$  to 0.09%  $X_0$ ), which influence, for example, the impact parameter resolution and tracking efficiency at low-transverse momenta.

In view of the future ALICE 3 detector, which consists of about 60 m<sup>2</sup> of MAPS sensors and is expected to be installed by 2035 at LHC, I will contribute to the design and construction of the first detector unit prototypes expected for 2027. The modules maintain a compact layout and an ultra-low material budget, while enabling fast data transmissions and powering over long distances. This requires the use of cutting-edge technologies such as the deposition of aluminium traces on dielectric substrates to form *Flexible Printed Circuits* (FPCs), which must be characterised mechanically and electrically to define viable integration solutions and must subsequently be validated through simulations of their impact on the detector performance. These FPCs can be then interconnected to the sensors through *TAB-bonding* and *flip-chip bonding* techniques, enabling modular and compact configurations that meet the ALICE 3 tracker requirements.

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Supervisor 1: Giacomo Contin

Supervisor 2: Paolo Camerini

Supervisor 3: David Novel

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
Quark Gluon Plasma: theory and experimental observations	Fragiacomo	2	16
The physics of imaging with X-rays and associate X-ray detectors	Menk/Brombal	3	24 (16 + 8)
Advanced data analysis techniques with machine and deep learning	Luparello	2	16
Introduction to RooFit	Pinamonti	2	16
		9	72

## AI in medical physics with a focus in Radiotherapy Maram S.K. Othman

### SUMMARY

*AI is spreading fast in the clinical medical physicist activity. In radiation therapy treatment planning there are a number of issues that that can be approached using AI to ensure the safety of the delivered dose to patient in different aspect related to the treatment delivered procedure starting from patient setup, organs contouring, and treatment verification dose lasting to delivering the dose with the appropriate and accurate way. Many published reviews emphasis on the advantages of AI in medical physics exercises that helps to improve in work flow for both physicist and patient care. Starting from the clinical needs of the CRO activity some of them will be exploited.*

### Project description

Radiotherapy workflow is a process that consists of several steps starting from patient imaging, treatment planning to dose-treatment delivering in such ways that many imaging modalities can be used, and numerous patient data need to be processed. This complete cycle of workflow is time-consuming but have impact on treatment quality verification and patient health outcome. Where proposing AI tools that can increase treatment quality, standardization and accelerate these steps leading to more safe, accurate and precise radiation treatment delivering when applying automation and optimization of workflow, to provide a personalized adaptive radiotherapy (ART). AI tools is characterized as a collection of algorithms that can perform tasks correlated with human thinking using machine learning (ML) and deep learning (DL). (see figure 1, ref 4)

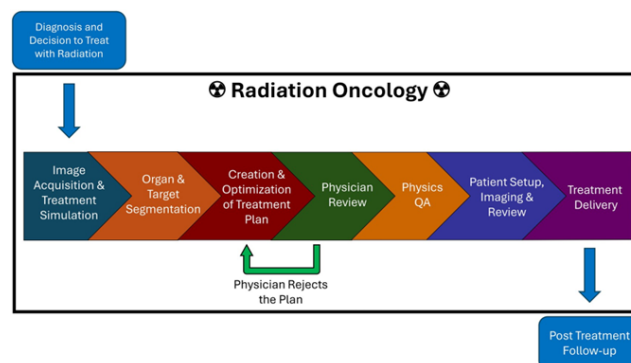


Figure 1 Radiotherapy clinical workflow for patients, ref 5

Artificial Intelligence (AI) that applied to medical images allows for automated disease detection, characterization of histology, stage, or subtype, and patient classification

according to therapy outcome or prognosis. It also permits outlining regions in the images, quantifying organ volumes, and extracting features from the images which, combined with machine learning algorithms, lead to quantification of image properties or image classification, distribution and delivered-dose verification image-based between different modalities. (see ref. 1)

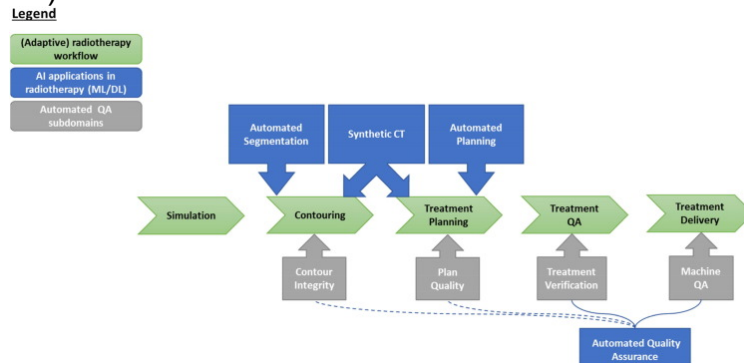


Figure 2 Artificial Intelligence implementation in Radiotherapy workflow, ref 4

The CRO oncological center in Aviano develops research activities mainly related to AI application in Organ Image segmentation, Image reconstruction and registration, Image artifact-free DL-based approach in MVCT-images in order to provide precise treatment dose calculation and calibration. CRO research activities also work on in-vivo EPID-image based treatment verification calibration for Adaptive Radiotherapy (ART) treatment and to inherit advanced dose verification system for patient-specific dosimetry. (Ref 2,3)

During the first year the candidate will cooperate with the active research in CRO, from the second year she will lead work package through CRO- clinical research project. Collaboration with the INFN research project in the field of AI in medicine is foreseen.

## **References:**

1. Michele Avanzo, Massimiliano Porzio, Leda Lorenzon, Lisa Milan, Roberto Sghedoni, Giorgio Russo, Raffaella Massafra, Annarita Fanizzi, Andrea Barucci, Veronica Ardu, Marco Branchini, Marco Giannelli, Elena Gallio, Savino Cilla, Sabina Tangaro, Angela Lombardi, Giovanni Pirrone, Elena De Martin, Alessia Giuliano, Gina Belmonte, Serenella Russo, Osvaldo Rampado, Giovanni Mettievier, Artificial intelligence applications in medical imaging: A review of the medical physics research in Italy, Physica Medica, Volume 83, 2021, Pages 221-241, ISSN 1120-1797, <https://doi.org/10.1016/j.ejmp.2021.04.010>.
2. Lorenzo Marini, Carlotta Mozzi, Aafke Kraan, Francesca Lizzi, Michele Avanzo, Alessandra Retico, Cinzia Talamonti, 2809 Artificial intelligence for in-vivo dosimetry using EPID in external beam photon radiotherapy, Radiotherapy and Oncology, Volume 206, Supplement 1, 2025, Pages S3406-S3408, ISSN 0167-8140, [https://doi.org/10.1016/S0167-8140\(25\)01304-0](https://doi.org/10.1016/S0167-8140(25)01304-0).



3. Carlotta Mozzi, Lorenzo Marini, Michele Avanzo, Aafke Kraan, Francesca Lizzi, Livia Marrazzo, Icro Meattini, Alessandra Retico, Cinzia Talamonti, 2826 Development and validation of a robust dataset using commercial TPS and radiochromic films for deep learning in transit dosimetry, Radiotherapy and Oncology, Volume 206, Supplement 1, 2025, Pages S2616-S2618, ISSN 0167-8140, [https://doi.org/10.1016/S0167-8140\(25\)01314-3](https://doi.org/10.1016/S0167-8140(25)01314-3).
4. Liesbeth Vandewinckele, Michaël Claessens, Anna Dinkla, Charlotte Brouwer, Wouter Crijns, Dirk Verellen, Wouter van Elmp, Overview of artificial intelligence-based applications in radiotherapy: Recommendations for implementation and quality assurance, Radiotherapy and Oncology, Volume 153, 2020, Pages 55-66, ISSN 0167-8140, <https://doi.org/10.1016/j.radonc.2020.09.008>
5. Kristen Duke, Nikos Papanikolaou, Artificial intelligence in radiation therapy: from imaging to delivery—a comprehensive review, BJR|Artificial Intelligence, Volume 2, Issue 1, January 2025, ubaf012, <https://doi.org/10.1093/bjrai/ubaf012>

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Supervisor 1: *Renata Longo*  
 Supervisor 2: *Michele Avanzo (CRO Aviano)*  
 Supervisor 3: *Fulvia Arfelli*

List of courses to be taken (pending confirmation)

Title	Teacher	CFU	Hours
The physics of imaging with x-rays and associated x-ray detectors	Ralph Menk/luca Brombal	3	
Bayesian statistics with numerical applications	Edoardo Milotti	3	
Simulation of particle interaction	Francesco Longo/Valentina Zacco	3	
Imaging with x-rays fundamental and applications	Pierre Thibault/Vittorio Tripani	2	
Advanced data analysis techniques with machine and deep learning	Grazia Luparello	2	
		<i>Insert total</i>	<i>Insert total</i>