

Candidate presentation

Candidate: Laria Figurato

Cycle: XXXVIII

Supervisor: Angelo Bassi

Co-supervisor: Matteo Carlesso, Sandro Donadi

Research Title: From Fuzzy Spacetime to Classical Reality

The Candidate has successfully accomplished the required educational activities as approved by the Teachers Board, including the Ph.D. courses, exams and the attendance of schools and conferences.

Brief description of the candidate research activity

The candidate's research explores the fundamental question of how gravity may influence the emergence of classical behavior from quantum mechanics, addressing one of the most intriguing open problems at the interface of these two foundational theories. The investigation develops along two complementary theoretical directions - gravitational decoherence and gravity-induced collapse - each offering a distinct mechanism by which gravitational effects could suppress or eliminate quantum superpositions.

In the first line of research, the candidate revisits and extends the Károlyházy model of gravitational decoherence, which attributes the loss of quantum coherence to stochastic fluctuations in spacetime geometry. Building upon this idea, a generalized stochastic framework has been developed to describe metric fluctuations in a self-consistent way, resolving inconsistencies present in earlier formulations and ensuring compatibility with current experimental constraints. This refined model quantifies how random gravitational potentials induce decoherence without invoking an explicit collapse of the wave function, thereby offering a purely dynamical mechanism for the apparent emergence of classicality. Through detailed analytical and numerical analysis, the candidate has delineated the parameter regimes in which such decoherence effects might become observable, providing concrete guidance for the design of future high-precision experiments.

The second research direction focuses on the Diósi–Penrose model, which proposes that the collapse of the wave function arises spontaneously due to the gravitational self-energy associated with spatial superpositions of mass distributions. Within this framework, the candidate has derived new theoretical bounds on the model's parameters by imposing consistency with the absence of macroscopic superpositions in everyday conditions. Furthermore, scaling relations for the collapse time have been systematically explored as functions of mass, geometry, and spatial dimensionality. The candidate has also extended the DP framework to incorporate non-Markovian (memory) effects, thereby capturing more realistic dynamics of gravitationally induced state reduction.

Taken together, these two lines of research establish a comparative picture of how gravity could act as a bridge between the quantum and classical realms — either through continuous stochastic decoherence or through objective wave-function collapse.

Role of the Candidate and main achievements.

The candidate has personally carried out the following research activities and achieved the following results, divided according to the two main lines of work:

Károlyházy Model – Gravitational Decoherence

- She developed a generalized stochastic framework to describe spacetime fluctuations, resolving inconsistencies present in previous formulations of the Károlyházy model.
- She ensured the model's consistency with current experimental bounds on metric noise and decoherence rates, refining its physical relevance.
- She quantified the loss of quantum coherence induced by stochastic gravitational potentials.
- She identified the parameter regimes in which gravitational decoherence could become experimentally observable, thus defining realistic experimental targets.

Diósi–Penrose Model – Gravity-Induced Collapse

- She performed the analytical and numerical study of the Diósi–Penrose model, linking spontaneous wave-function collapse to the gravitational self-energy of mass distributions.
- She derived new upper bounds on the collapse parameters by imposing consistency with the absence of macroscopic quantum superpositions in everyday conditions.
- She analyzed the scaling behavior of collapse times as functions of mass, geometry, and dimensionality, revealing how gravitational effects influence state reduction.
- She extended the Diósi–Penrose framework to include non-Markovian (memory) effects, providing a more realistic dynamical description of gravitational collapse.
- She conducted a comparative analysis between gravitational decoherence and objective collapse, highlighting their conceptual and phenomenological differences.

This research has led to the publication of two papers, both with the candidate as first author.

General evaluation of the candidate by the supervisor

I consider Laria's overall performance to be good. She has been consistently enthusiastic and hard-working, and she has brought several tasks to completion. She's always been very collaborative and engaged with the research group. At the same time, her progress required closer supervision than is typically expected of a PhD candidate at this stage. Her scientific writing and command of English are adequate but not strong, and her manuscripts benefited from substantial editorial input. She has produced two publications; while this is acceptable, usually students achieve a higher output. In summary, Laria has delivered solid work and shown commitment, even if her results and level of autonomy do not place her among the strongest students I have supervised.

Summary: The Teachers Board agrees that the candidate fully achieved the training and scientific targets set at the beginning of the Ph.D. program

Presentations to Conferences, workshops, and meetings

TALKS:

- On the effectiveness of the collapse in the Diósi–Penrose model
Workshop “DICE2024”(2024)
- On the effectiveness of the collapse in the Diósi–Penrose model
Doctoral school “Fundamental problems in quantum physics 2024” (2024)
- On the effectiveness of the collapse in the Diósi–Penrose model
Workshop “A look at the interface between gravity and quantum theory - 2024 edition”(2024)
- On the effectiveness of the collapse in the Diósi–Penrose model
Workshop “Modern odyssey: quantum gravity meets quantum collapse at atomic and nuclear physics energy scales in the cosmic silence”(2024)
- On the testability of the Károlyházy model
Doctoral school “Fundamental problems in quantum physics 2023”(2023)
- On the testability of the Károlyházy model
Workshop “A look at the interface between gravity and quantum theory”(2023)

SEMINARS:

- “On the testability of the Károlyházy model ”
Seminar given to the QMTS group, University of Trieste
- “On the effectiveness of the collapse in the Diósi–Penrose model”
Seminar given to the QMTS group, University of Trieste

LECTURES:

- “Italian Quantum Weeks”, “giovani quantistici @trieste”, (Gorizia, 2023)
Invited lecturer

POSTERS:

- “Emergence of classicality: new perspectives on measurements in quantum theory”(2024) best poster prize

Publications

- L. Figurato et al., New J. Phys. **26** 113004 (2024), “On the effectiveness of the collapse in the Diósi–Penrose model”
- L. Figurato et al., New J. Phys. **26** 013001 (2024), “On the testability of the Károlyházy model”

Candidate presentation

Candidate: Giovanni NICHELE

Cycle: XXXVIII

Supervisor: Fabio BENATTI

Co-supervisor: Angelo BASSI

Research Title:

On the Classical and Quantum Aspects of Memory Effects in Open Dynamical Systems

The Candidate has successfully accomplished the required educational activities as approved by the Teachers Board, including the Ph.D. courses, exams and the attendance of schools and conferences.

Brief description of the candidate research activity

The candidate research activity has developed along three main lines, with the overall purpose of comparing and contrasting classical and quantum non-Markovian stochastic processes. A central concept throughout the thesis has been the so-called backflow of information (BFI) that may occur in quantum dynamics with memory effects both classically and quantum mechanically.

i. Classical Reduction of Quantum Dynamics.

The first aspect studied by the candidate was the restriction of a quantum dynamical process to any fixed maximally Abelian (i.e. commutative) subalgebra that yields a classical stochastic process.

ii. Superactivation of Memory Effects.

The second issue addressed by the candidate was the study of quantum memory effects with no classical counterpart as when two independently evolving parties that do not show BFI when considered independently, do so when statistically coupled.

iii. Dynamical Entropy and non-Markovianity.

The third issue addressed by the candidate was the study of the physical mechanisms underlying memory effects. These are extremely difficult to assess if using the reduced dynamical map only. The latter is indeed just the one-time marginal of an underlying stochastic process. As a consequence the candidate studied the Alicki–Lindblad–Fannes dynamical entropy for open systems, **that can be computed by means of the multi-time statistics.**

Role of the Candidate and main achievements.

Regarding all three research lines, Giovanni Nichele has demonstrated a truly remarkable level of scientific independence, physical vision and technical skills.

i. Classical Reduction of Quantum Dynamics ([2]).

If the original process is P-divisible, the classically reduced process need not be such, the typical example being that of a unitary evolution. Conversely, for some paradigmatic examples of purely dissipative processes, Nichele showed

that P-divisibility is preserved by the classical reduction. The main finding has been the construction of a purely dissipative quantum evolution whose classical restriction loses P-divisibility. The corresponding classical revivals of distinguishability have been called superactivation of BFI (SBFI) then interpreted as quantum coherence-assisted BFI, in full analogy with the open-system scenario

ii. **Superactivation of Memory Effects ([1,3,4]).**

SBFI has been shown to occur via the coupling of a quantum system to a classical stationary environment, as for two qubits each coupled to a classical Markov chain [3]. The study of SBFI led to (a) its phenomenological characterization through quantum correlations (beyond entanglement); (b) a constructive way to witness SBFI in terms of entropic quantities [4]; (c) its physical characterization in terms of the growth and collapse of system–environment correlations [3].

iii. **Dynamical Entropy and non-Markovianity.**

The candidate computed exactly the ALF entropy for the collisional model described in point ii. and further provided an example of zero dynamical entropy, mimicking the behavior of a reversible evolution, though in presence of an open irreversible quantum dynamics. The ALF entropy has also been operationally interpreted through the state-purification scheme provided by the GNS construction: in such a context a link between the quantum dynamical entropy and the SBFI effect naturally emerged.

General evaluation of the candidate by the supervisor:

Giovanni Nichele certainly proved my best PhD student ever. His redoubtable technical skills made him rapidly acquainted with the techniques of algebraic quantum statistical mechanics so that he could soon independently work his way through the problems I proposed him which required a variety of both mathematical and physical insights.

The interesting results he obtained in relation to the time-behaviour of entropy and correlations in open quantum dynamics with memory effects are very interesting and led to four publication plus certainly one, maybe two, papers in preparation.

It has been a real pleasure to work with Giovanni Nichele, also because of his personal calm character as a human being and his willingness to listen and learn. I am firmly convinced that, if he so wishes, a bright scientific future awaits him.

Summary: The Teachers Board agrees that the candidate fully achieved the training and scientific targets set at the beginning of the Ph.D. program

Presentations to Conferences, workshops, and meetings

1. **INVITED TALK** - “N_O_N_-MARKOVIAN OPEN QUANTUM SYSTEMS AND DYNAMICAL ENTROPY: A COLLISIONAL MODEL PERSPECTIVE” _56 SYMPOSIUM ON MATHEMATICAL PHYSICS, INSTITUTE OF PHYSICS, TORUŃ (POLAND), JUNE 2025, ABSTRACT AVAILABLE AT https://fizyka.umk.pl/smp/smp56/Abstr_56T.pdf
2. **CONTRIBUTED TALK** - “NON_MARKOVIAN OPEN QUANTUM SYSTEMS AND DYNAMICAL ENTROPY: A COLLISIONAL MODEL PERSPECTIVE” – IQIS2025, BOLOGNA, SEPTEMBER 2025, ABSTRACT AVAILABLE AT https://events.unibo.it/iqis-2025/conference-program/booklet_finale-2.pdf/@@download/file/BOOKLET_FINALE-4.pdf
3. **CONTRIBUTED TALK** – “SUPERACTIVATION OF BACKFLOW OF INFORMATION IN A CLASSICAL MARKOV ENVIRONMENT”, 111° CONGRESSO SIF, PALERMO, SEPTEMBER 2025, ABSTRACT AVAILABLE AT https://static.sif.it/SIF/resources/public/files/congr25/atti-congresso-111_2025.pdf

Publications

1. F. BENATTI, G. NICHELE, OPEN QUANTUM DYNAMICS: MEMORY EFFECTS AND SUPERACTIVATION OF BACKFLOW OF INFORMATION, *MATHEMATICS* 12, 37.(2024) <https://doi.org/10.3390/math12010037>
2. F. BENATTI, D. CHRUSCINSKI, G. NICHELE (2024). QUANTUM VERSUS CLASSICAL P-DIVISIBILITY. *PHYSICAL REVIEW A*, 110(5), 052212. (2024) <https://doi.org/10.1103/physreva.110.052212>
3. F. BENATTI, G. NICHELE, SUPERACTIVATION OF MEMORY EFFECTS IN A CLASSICAL MARKOV ENVIRONMENT. *PHYSICA SCRIPTA*, 100(6), 065115. (2025) <https://doi.org/10.1088/1402-4896/add57e>
4. G. NICHELE, F. BENATTI, ENTROPIC SUPERACTIVATION OF BACKFLOW OF INFORMATION. *QUANTUM ECONOMICS AND FINANCE*, FIRST ONLINE, (2025). <https://doi.org/10.1177/29767032251361881>

Candidate presentation

Candidate: Ivaldevigles Rodrigues De Souza Junior

Cycle: XXXVIII

Supervisor: Andrea Trombettoni

Co-supervisor: Carla Braitenberg

Research Title: Quantum Gravimeters for Geophysical Applications

The Candidate has successfully accomplished the required educational activities as approved by the Teachers Board, including the Ph.D. courses, exams and the attendance of schools and conferences.

Brief description of the candidate research activity

This doctoral research focused on the modeling, simulation, and geophysical applications of quantum gravimeters. It first developed detailed descriptions of two- and three-level atomic systems, emphasizing atom–light interactions and the basic principles of atomic interferometry. The role of $\pi/2$ and π Raman pulses in Mach–Zehnder interferometers was analyzed, linking the accumulated phase difference to local gravitational acceleration. The study also examined the influence of pulse temporal shapes and provided an in-depth analysis of the sensitivity function, used to characterize noise sources affecting the interferometer. The analyses highlighted how the Rabi frequency and pulse duration determine atomic state transitions and the resulting interferometric response. The core research activities involved numerical simulations based on synthetic data for two models of geophysical interest. A split-operator method was used to model the temporal evolution of the probability density function, enabling assessment of pulse-phase effects on final measurements and of phase accumulation along atomic trajectories under acceleration. Finally, computational geophysics techniques were applied to generate synthetic gravimetric anomalies and evaluate the ability of quantum gravimeters to detect subsurface heterogeneities. Inversion methods such as Tikhonov regularization and the generalized inverse were used to estimate density distributions, supporting the assessment of quantum gravimeters for four-dimensional monitoring in fluid-substitution scenarios.

Role of the Candidate and main achievements.

The PhD candidate began the program with a strong and advanced background in geophysics, but with only limited prior exposure to quantum mechanics and the theoretical tools required for the study of quantum sensors and quantum gravimeters.

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For this reason, the initial phase of the doctoral work focused on strengthening his background in quantum mechanics, atomic physics, and atom–light interaction. This period of training and self-study was carried out with diligence and led to a good understanding of the concepts necessary for the subsequent stages of the project.

Once this formative phase was successfully completed, the candidate was able to approach the assigned research topics with increasing autonomy. He applied the newly acquired theoretical knowledge to the modeling and simulation of quantum gravimeters. Throughout the project he maintained a high level of dedication, producing good scientific results and showing a growth in both his technical skills and his ability to work independently. It is important to underline that combining competencies in both geophysics and quantum mechanics is challenging in our opinion and (at date) relatively uncommon. Developing expertise across these two domains requires considerable effort, but it also provides a valuable “plus” in the rapidly evolving field of quantum technologies. We therefore acknowledge not only the difficulty of the path undertaken, but also the significance of successfully integrating these skill sets.

General evaluation of the candidate by the supervisor:

The candidate has worked with strong dedication throughout the entire project. Over time, he has increased his level of autonomy, taking greater responsibility for both the theoretical and computational aspects of his research. His progress reflects not only a technical growth but also a capacity to work on quantum sensors independently and to contribute actively to the advancement of the project.

Summary:

The main challenge of the Ph.D. project was to combine, on the basis of the PNRR NQSTI-Spoke 3 proposal (funding the fellowship), an operative knowledge of the microscopic working principle of ultracold quantum gravimeters with the ability to be able to work on concrete technological applications, and in particular geophysical ones. The Teachers Board agrees that the candidate achieved the needed training and level of skills from theory of quantum devices and geophysics and reached the scientific targets set at the beginning of the Ph.D. program.

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Presentations to Conferences, workshops, and meetings

Since the main research work that will form the basis of his thesis has been not yet submitted, the candidate has not yet given conference presentations. However, he gave two presentations of his on-going work, one at a School in Grenoble (March 2024) and one at University of Florence (march 2025), where he interacted with the group of Prof. Guglielmo Tino and Dr. Gabriele Rosi, a leading group in the field of ultracold quantum gravimetry.

Publications

Two research articles based on his doctoral work are currently approaching completion. The plan is to finalize these manuscripts and submit them for publication prior to the PhD defense.

Candidate presentation.

Candidate: Alessandro Namar

Cycle: XXXVIII

Supervisor: prof. Erik Vesselli

Co-supervisor: dr. Mattia Scardamaglia (MAX IV – Lund University – Sweden)

Research Title: Structure and reactivity of biomimetic iron-centered 2D materials from ultra-high vacuum to near-ambient pressure.

The Candidate has successfully accomplished the required educational activities as approved by the Teachers Board, including the Ph.D. courses, exams, the attendance of schools and conferences, and a six-months period spent abroad.

Brief description of the Candidate research activity.

The experimental research activity of the Candidate was focused on the growth and characterization in Ultra High Vacuum (UHV) conditions of iron-based self-assembled metal-organic monolayers at surfaces, associated with the investigation of their reactivity to small gases up to near ambient pressure. Specifically, self-assembly, trans-metalation and ligation processes were investigated. The peculiarity of the project consisted in the need to exploit combinations of several complementary experimental surface science techniques to both grow and investigate the systems of interest. The Candidate used not only standard state-of-the-art surface science methods, but also the most recent approaches to allow a detailed atomic level description beyond the UHV constraints of conventional probes. Thus, in addition to *in vacuo* methods like STM, NEXAFS, and XPS, he exploited IR-Vis SFG, PM-IRRAS and AP-XPS intensively, yielding a thorough atomic-level insight into the electronic, chemical, and geometrical properties of the heterostacks. Experiments were performed both at laboratories and synchrotron radiation facilities.

Role of the Candidate and main achievements.

The Candidate worked in the framework of an international collaboration network, including experimental and computational contributors. This point was crucial due to the necessity of a multi-technique approach to the characterization of the new materials. The Candidate acted as principal investigator in his project, participating in and leading the measurement sessions (Trieste, Lund, Graz, Barcelona) and the data analysis and interpretation workflows, together with the interaction with the computational counterpart (Udine). The methods, combined with the innovative 2D materials that were investigated, based on a substantial biomimetic approach, yielded unprecedented results that deserved (and will deserve) publication in high-impact factor peer-reviewed journals. In brief, the main achievements consisted in:

- *Iron and iron-cobalt porphyrin networks.*
 - *Synthesis and characterization.* Cobalt-driven self-assembly of iron tetra-

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pyridyl-porphyrins on graphene, with formation of coordination-dependent long-range ordered superstructures and control of the metals' oxidation states.

- *Reactivity.* Reactivity of the Co and Fe centers at room temperature at ambient pressure towards carbon monoxide and oxygen; investigation of non-local effects affecting carbonylation and of the di-oxygen activation mechanisms.
- *Hemin*
 - *Deposition and layers growth.* Layers geometric and electronic structure, role of the residual carboxylic terminations, molecular overlapping, un-metalated species.
 - *Trans-metalation.* Co dosing and synthesis of cobalt protoporphyrin surface species.
 - *Reactivity.* Di-oxygen activation and oxygen-assisted trans-metalation mechanisms at near-ambient pressure conditions.

General evaluation of the Candidate by the supervisor:

Supervisor's evaluation:

The project assigned to the Candidate was experimentally very challenging from at least three points of view. First: the synthesis recipes of the 2D heterostacks needed to be tuned. Second: the characterization methods to yield ambient pressure insight are tricky to use, especially IR-Vis SFG. Third: the interpretation of the rough spectroscopic data was not straightforward and deep insight into literature and cross-correlation of the available experimental information was crucial, together with corroboration with additional experimental approaches. Within the framework of the PhD program, the Candidate became very independent, being able to design experiments, analyze the data, and provide an interpretation picture with adequate scientific criticism. Meanwhile, he also co-supervised a few Master students during their theses and training activities. He took part at several beamtimes allocated through peer-reviewed, highly competitive access calls at international synchrotron radiation sources throughout Europe. Thus, I think that he represents an excellent Candidate to be awarded the PhD title in Physics.

Co-supervisor's evaluation:

Having known the Candidate already before the six-month period, I can say that he has shown remarkable growth during this time, becoming more mature and independent. He provided valuable support at the beamline, successfully carrying out tasks beyond the direct scope of his PhD project. With the aim of mastering the APXPS experimental technique, he also voluntarily participated in two beamtimes of our team that were not directly related to his Thesis work, where he proved to be a reliable and effective contributor, as testified by co-authoring a scientific publication.

In general, he demonstrated the ability to adapt and integrate well into a new group and into an international and dynamic work environment such as a synchrotron facility.

Within a short time, he was able to handle complex beamline experiments, overcoming his initial uncertainty. He has been proactive and constructively critical, both in managing his experimental work and in the analysis and interpretation of the data.

Overall, I consider him a motivated and competent researcher, well-prepared to complete the PhD.

Summary:

In summary, the Teachers Board agrees that the Candidate fully achieved the training and scientific targets set at the beginning of his Ph.D. program.

Presentations to Conferences, workshops, and meetings

- Spectroscopy Summer School @Max IV, Lund, 21st-25th August 2023, poster presentation: “An *in situ* spectroscopic and vibrational surface characterization of a protein’s solvation: the case of vitamin B12/Au(111)”
- ECSCD-16/ICSOS-14 Conference in Wien with oral presentation entitled: “Cooperativity in a graphene-supported FeTPyP-Co metalorganic network: the role of electronic and geometric structure.”
- APXPS 2025, New York, 8th-12th December 2025, poster presentation: “Bio-inspired Surface Catalysis: Hemin Reactivity”

Beamtimes

- MAX IV – HIPPIE beamline
 - ID 20221030 “Self-metalation of tetrapyrroles at the gas-solid interface.” (09/05/2023-15/05/2023)
 - ID 20230232 “2D bio-mimetic materials towards the second coordination sphere: an *in situ* spectroscopic characterization of the active site ligation environment in a synthetic cobalamin-based 2D material.” (20/02/2024-26/02/2024)
 - ID 20231733 “Studying subsurface carbon segregation in a palladium catalyst during methane oxidation” (21/05/2024-27/05/2024)
 - ID 20231301 “Cooperativity effects in a FeTPyP-Co metalorganic framework on graphene: the role of electronic configurations and local coordination.” (12/06/2024-17/06/2024)
 - ID 20240738 “Self-sustained oscillations studied with new tr-APXPS methods”. (28/08/2024-02/09/2024)
 - ID 20240093 “From 2D metalorganic frameworks to the second coordination sphere: reactivity of one-armed porphyrins at surfaces.”. (23/10/2024-28/10/2024)
 - ID 20241097, in house research, “Cooperativity effects in a FeTPyP-Co metalorganic framework on graphene: the role of electronic configuration and local coordination. (15/10/2024-20/10/2024)
- MAX IV – FlexPES beamline
 - ID 20240091 “From 2D metalorganic frameworks to the second coordination sphere: electronic and geometric structure of one-armed porphyrins at surfaces” (02/10/2024-07/10/2024)

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- ALBA – BOREAS beamline
 - ID 2024028422, "Ferromagnetism on 2D bimetallic organic frameworks", at beam line BL29 - BOREAS (18/09/2025-21/09/2025)

Periods abroad

- MAX IV – Lund University – Sweden: 01/05/2024-01/11/2024
- Graz University – Austria: 29/06/2025-04/07/2025

Publications

- U. Küst, R. Jones, J. Prumbs, A. Namar, M. Scardamaglia, A. Shavorskiy, J. Knudsen, "Carbon subsurface traffic jam as driver for methane oxidation activity and selectivity on Palladium surfaces": *Nat. Commun.* **16** (2025) 7755, DOI: 10.1038/s41467-025-63088-9.
- S. Baronio, M. De Col, A. Yadav, B. Roondhe, V. Mischke, O. Resel, D. Bidoggia, A. Namar, N. Vinogradov, M. Scardamaglia, M. Valvidares, P. Gargiani, M. Cinchetti, G. Zamborlini, P. Giannozzi, E. Vesselli, "Single atom coordination in a manganese-cobalt bi-metallic framework on graphene: geometric and electronic structures": *Nanoscale* **17** (2025) 16946, DOI: 10.1039/D5NR01383F.
- A. Yadav, S. Baronio, M. De Col, D. Comini, V. Mischke, A. Namar, N. Vinogradov, M. Scardamaglia, M. Cinchetti, G. Zamborlini, P. Giannozzi, E. Vesselli, "Pressure-controlled oxygen activation at single metal atom sites in a manganese-cobalt coordination network on graphene: from triplet-singlet spin transition to superoxo dissociation": *submitted*.
- M. De Col, D. Comini, S. Baronio, B. Roondhe, A. Namar, D. Bidoggia, M. Scardamaglia, P. Giannozzi, E. Vesselli, "Carbon monoxide ligation at single metal atom sites in a 2D manganese-cobalt coordination network: equilibrium at room temperature": *in preparation*.
- A number of papers (3-4) will be drafted after completion of the Candidate's PhD program, since corroborating data analyses and DFT calculations are still running.

Candidate presentation

Candidate: Alice Damiano

Cycle: XXXVIII

Supervisor: Stefano Borgani

Co-supervisor: Milena Valentini

Research Title: Tracing Supermassive Black Holes in Cosmological Simulations

The Candidate has successfully accomplished the required educational activities as approved by the Teachers Board, including the Ph.D. courses, exams and the attendance of schools and conferences.

Brief description of the candidate research activity

Alice's research has primarily focused on investigating the evolution of massive black holes (MBHs) in cosmological simulations of structure formation. In particular, her work explored the impact of unresolved dynamical friction (DF) on the dynamics of MBH particles in such simulations. Because of the limited mass and force resolution inherent in cosmological N-body and hydrodynamical codes, the N-body gravity solver cannot accurately capture the effect of dynamical friction MBH particle exerted by the surrounding distribution of stars and dark matter (DM). This limitation affects the orbital decay and merger timescales of MBH pairs, especially in cases where the MBH masses are comparable to or smaller than the mass of nearby stellar or DM particles. This long-standing issue has been addressed by various groups using different approaches.

Remarkably, Alice conceived, developed, and implemented in the `OpenGADGET3` code a relatively simple yet highly effective scheme to correct MBH orbits for the unresolved DF component. She carried out extensive tests - both in fully cosmological simulations and in controlled numerical experiments - to assess the validity of her DF model across different resolutions, environments, and evolutionary stages. Furthermore, she compared her implementation against alternative DF treatments from the literature, demonstrating its superior ability to reproduce realistic MBH orbital decay within simulated galaxies and to recover inspiral timescales consistent with analytical predictions even at modest numerical resolution. In addition, through an analytical derivation, Alice showed that the DF correction she proposed can be identified with the first-order diffusion term of the Fokker-Planck equation describing the evolution of a self-gravitating system. This elegant connection provides a solid theoretical foundation for her numerical approach.

The DF correction model developed by Alice has now been adopted as the **default treatment** for unresolved dynamical friction within the `OpenGADGET3` code.

Alice presented the results of this work in **two first-author papers**, both published in *Astronomy & Astrophysics*.

In a separate project, Alice performed and analysed an extensive suite of cosmological hydrodynamical simulations of galaxy clusters and groups with `OpenGADGET3` to investigate different aspects of MBH evolution — including seeding, accretion, and merging - and the

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resulting AGN feedback. This study led to another first-author paper, which has been submitted to *Astronomy & Computing* and is currently under review.

Role of the Candidate and main achievements.

Although Alice's PhD project was carefully planned and regularly discussed with her supervisors, she maintained full control and responsibility for the code development related to the implementation of the dynamical friction (DF) correction model, the execution of both test and production simulations, and the analysis of the resulting data - including the development of a significant portion of the post-processing software.

At every stage of the project, Alice took a leading and proactive role in shaping and refining its scientific direction from the early phases of her PhD. She showed remarkable independence in developing her own original ideas for the DF model and in defining a comprehensive campaign of controlled numerical simulations to test it in detail.

Alice also prepared and submitted several proposals for supercomputing time - including an ISCRA-B proposal at CINECA - all of which were successfully awarded. She consistently took full responsibility for the first interpretation of simulation results and demonstrated a high level of critical judgment. While she regularly reported progress to her supervisors, she seldom needed to seek guidance, even when facing unexpected outcomes or technical difficulties.

By the end of her PhD, Alice had achieved full mastery of the black-hole and AGN modules within the OpenGADGET3 code - a significant accomplishment for a PhD student, given the complexity of this software.

Alice also spent three months as a visiting PhD student at the University of Zurich, joining an active group with strong expertise in simulations of black hole dynamics. During this visit, she became familiar with the Changa simulation code used by that group, implemented her DF model within it, and initiated a new collaboration on the evolution of massive black hole pairs during galaxy-galaxy mergers. The results of this work are at an advanced stage but not yet finalized, and thus are not included in her thesis.

Finally, Alice independently established a collaboration with the IT4I Institute at the University of Ostrava (Czech Republic), aimed at developing advanced visualization techniques for cosmological simulations.

General evaluation of the candidate by the supervisor:

Alice has been an excellent PhD student from the very beginning of her doctoral studies. From the outset, she demonstrated a strong aptitude for independent scientific thinking, combined with enthusiasm, genuine curiosity, and a highly collaborative attitude. She has consistently shown great care in preparing presentations for group meetings, journal clubs, and progress reports, with a level of thoroughness and clarity that is uncommon among early-stage PhD students. In all professional interactions, Alice has proven to be reliable, thoughtful, and efficient. She takes the initiative to investigate issues in depth before asking for guidance, ensuring that discussions with her are focused, productive, and intellectually stimulating.

Highly self-motivated and meticulous, Alice is an independent and critical thinker who rigorously checks her own work and systematically investigates any potential sources of

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uncertainty. She engages actively and constructively in scientific discussions, both with her collaborators and with other colleagues, always seeking to gather different perspectives and to address challenging or controversial aspects of the problem. When discussing her work, she clearly articulates her reasoning and supports her conclusions with well-founded arguments. She also approaches suggestions and feedback with genuine interest, reflecting a strong commitment to learning and improving. Throughout her PhD, Alice has successfully navigated both the steep technical learning curve and the conceptual complexities involved in disentangling genuine astrophysical effects from numerical artifacts in sophisticated cosmological simulations.

During her time in Trieste and through her participation in international conferences and her three-month visit at the University of Zurich, Alice has established several productive collaborations with researchers working on related topics. Her enthusiasm and openness make her interactions with both senior and junior colleagues particularly engaging and effective.

Alice has been diligent and precise in the preparation of her manuscripts. Her presentations at international conferences - several of which were invited - were always clear, well-structured, and delivered with confidence. They frequently stimulated lively discussions, which she handled with professionalism and intellectual maturity. Beyond her individual research, Alice has also been an active and valuable member of the scientific community within her group and institute.

In summary, Alice has successfully completed all aspects of her PhD work and has clearly made the transition from a student to an independent, professional, and highly skilled researcher.

Summary: The Teachers Board agrees that the candidate fully achieved the training and scientific targets set at the beginning of the Ph.D. program

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Presentations to Conferences, workshops, and meetings

- 24th May 2023 - PhD and PostDoc seminars, Astronomical Observatory of Trieste (Italy). Contributed talk.
- 13th June 2023- INAF- Spoke 3 General Meeting University of Catania (Italy). Contributed talk.
- 15th June 2023 - INAF-USC VIII Workshop, University of Catania (Italy). Contributed talk.
- 14th July 2023 - Hydrosim meeting Sexten Center for Astrophysics, Sesto (Italy). Contributed talk.
- 14th September 2023 - Conference of the Italian Physical Society, University of Salerno, Fisciano (Italy). Invited talk.
- 16th October 2024 - The problematic existence of massive black holes at $z > 6$. Workshop at ICTP (Trieste). Invited talk.
- 13th July 2024 - The origin of Supermassive Black Holes Sesto (Italy). Contributed talk.
- 28th July 2024 - The OpenGadget3 code meeting. Lubijana (Slovenia) Contributed talk.
- 5th May 2024 - Spoke3 General Meeting, Isola d'Elba (Italy). Attendant.
- 4th June 2024 - HPC INAF School for Astrophysics, Bologna (Italy). Attendant
- 24th April 2025 – MiaPbP workshop on Active Galactic Nuclei, Munich (Germany). Contributed talk.
- 26th May 2025 – Spoke3 Technical Meeting, Perugia (Italy). Contributed talk.
- 1st September 2025 - Young Astronomers on Active Galactic Nuclei, Southampton (England). Contributed talk.

Publications

Damiano A., Valentini M., Borgani S., Tornatore L., Murante G., Ragagnin A., Ragone-Figueroa C., Dolag K., "[Dynamical friction and the evolution of black holes in cosmological simulations: A new implementation in OpenGadget3](#)", A&A, **Volume** 692, December 2024

Damiano A., Borgani S., Valentini M., Murante G., Tornatore L., Strakos P., Jaros M., "[Dynamical friction and massive black hole orbits: analytical predictions and numerical solutions](#)", accepted for publication on Astronomy&Astrophysics

Damiano A., Borgani S., Murante G., Valentini M., Tornatore L., Taffoni G., "Numerical solutions for black hole feeding and feedback in cosmological simulations with OpenGADGET3", submitted for the publication to Astronomy & Computing

Candidate presentation

Candidate: Marius Daniel Lepinzan

Cycle: XXXVIII

Supervisor: Pierluigi Monaco

Co-supervisors: Luca Tornatore, Tiago Batalha de Castro

Research Title: Advancing cosmological simulations with GPU-enabled PINOCCHIO: from dark matter halos to cosmic voids

The Candidate has successfully accomplished the required educational activities as approved by the Teachers Board, including the Ph.D. courses, exams and the attendance of schools and conferences.

Brief description of the candidate research activity

The candidate has worked on the development and scientific exploitation of the PINOCCHIO code for fast cosmological simulations. His work has developed along two directions.

(1) Code development: the first part of the PINOCCHIO code, that in origin required 70% to 90% of the computing time, has been ported to the GPUs, with dramatic speed-up of a factor of >10 (depending on the architecture) and similar advantage in terms of time-to-solution and energy-to-solution. As a result, the first part now requires $<10\%$ of the computing time. The second part of the code is harder to parallelize, an investigation on how to transform it using machine learning tools has led to interesting but still inconclusive results, so that its parallelization remains a work in progress.

(2) Code exploitation: the candidate has tested the accuracy with which PINOCCHIO is able to recover the statistics of cosmic voids, to be used as a powerful cosmological tool. The test has been carried out by analysing standard N-body simulations and PINOCCHIO runs performed on the same initial conditions. Four commonly used summary statistics, based on voids traced by dark matter halos, have been analysed, and good agreement was found in all cases. The resulting paper paves the way to the cosmological exploitation of Pinocchio mock galaxy catalogues by the void community. Furthermore, the candidate participated in an Euclid paper presenting an extended set of simulated spectroscopic samples, run with PINOCCHIO, and, as a side project, to the development of a deblending algorithm for Euclid image analysis.

Role of the Candidate and main achievements.

The candidate has carried out the part of code development and GPU porting with great autonomy. The first step, the porting the embarrassingly parallel computation of collapse times to GPUs, required the re-writing of low-level algorithms of bilinear and spline interpolation, since the Gnu Scientific Library used for these steps has not been ported to GPUs. This was done in total autonomy and with method. The rest of the work was done in collaboration with the group at INAF-OATs (especially Giovanni Lacopo and David Goz), where the role of the candidate has soon changed from implementation to

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coordination.

For the parallelization of the second part of the code, the candidate proposed to use a clustering algorithm that he was developing for deblending images as a base to identify halos in the Lagrangian space. This allowed our group to change perspective on the problem and investigate new roads to achieve a satisfactory parallelization. This work, which is much more complex than the previous one, has not converged yet, but we plan to carry it on in the next year.

The idea of investigating voids was suggested by the candidate himself, as a relevant application of PINOCCHIO that was never done before (we were concentrated on galaxies and galaxy clusters). This project was carried out in collaboration with the group of Joe Mohr in Munich. The candidate has done most of the work, from running OpenGadget-3 simulations and PINOCCHIO runs, to analysing the results and finding the best way to show them in the paper.

The candidate has become the main maintainer of the github repository of the PINOCCHIO code. As such, his contribution to the Euclid paper, PI-ed by P. Monaco, has been moderate, but sufficient to gain a position in the first tier of lead authors.

The side project of deblending of Euclid images was carried out within Euclid Science Ground Segment, where he took lead of a new deblending code to be used for the future Data Release 2.

General evaluation of the candidate by the supervisor:

Being funded by ICSC/Spoke 1, this project had the ambition of moving along two parallel tracks, from hard-core code development to science exploitation. The candidate succeeded in carrying out a thesis that presents significant contributions to both tracks, and at the same time to lead a task within the large Euclid collaboration. From this point of view, the fact that the parallelization of the second part of the code was not completed is a minor problem with respect to the amount of work he has collected in these three years.

The strong points of the candidate are his autonomy, his technical skills and his effective communication, that make him in a position to propose a problem, address it and present it in a clear and pleasant way.

Summary:

The Teachers Board agrees that the candidate fully achieved the training and scientific targets set at the beginning of the Ph.D. program

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Presentations to Conferences, workshops, and meetings

- TECHNICAL MEETING SPOKE 3, OCTOBER 9-11, 2023, UNIVERSITÀ DEGLI STUDI DI TRIESTE PIAZZALE EUROPA 1, [HTTPS://INDICO.ICT.INAF.IT/EVENT/2532/](https://indico.ict.inaf.it/event/2532/)
- SPOKE3 - MONTHLY WP1-2 MEETING, ONLINE, [HTTPS://INDICO.ICT.INAF.IT/EVENT/2744](https://indico.ict.inaf.it/event/2744)
- UNiVERSUM, FEBRUARY 21-23, 2024, SAPIENZA UNIVERSITÀ DI ROMA, PIAZZALE ALDO MORO, 5, [HTTPS://DOCS.GOOGLE.COM](https://docs.google.com)
- SPOKE3 GENERAL MEETING, MAY 05-09, 2024, HOTEL HERMITAGE, ISOLA D'ELBA, [HTTPS://INDICO.ICT.INAF.IT/EVENT/2752](https://indico.ict.inaf.it/event/2752)
- CLUSTER4, SEPTEMBER 10-13, 2024, UNIVERSITÀ DI TRIESTE, TRIESTE, [HTTPS://SITES.GOOGLE.COM/VIEW/CLUSTER4TS/](https://sites.google.com/view/cluster4ts/)
- TECHNICAL MEETING SPOKE 3, DECEMBER 17-19, 2024, RESEARCH AREA OF BOLOGNA, BOLOGNA, [HTTPS://INDICO.ICT.INAF.IT/EVENT/3001/](https://indico.ict.inaf.it/event/3001/)
- TECHNICAL MEETING SPOKE 3, MAY 26-29, 2024, HOTEL GIÒ JAZZ & WINE, PERUGIA, [HTTPS://INDICO.ICT.INAF.IT/EVENT/3173/](https://indico.ict.inaf.it/event/3173/)

Publications

- LEPINZAN ET AL. (2025). "TRACING COSMIC VOIDS WITH FAST SIMULATIONS". A & A, ACCEPTED FOR PUBLICATION ([ARXIV:2506.19506](https://arxiv.org/abs/2506.19506))
- LEPINZAN ET AL. (2025). "ACCELERATING COSMOLOGICAL SIMULATIONS ON GPUS: A PORTABLE APPROACH USING OPENMP". A & C, SUBMITTED TO "VSI: HPC IN COSMOLOGY AND ASTROPHYSICS" SPECIAL ISSUE ([ARXIV:2510.02873](https://arxiv.org/abs/2510.02873))
- LACOPO, LEPINZAN ET AL. (2025). "ACCELERATING COSMOLOGICAL SIMULATIONS ON GPUS: A STEP TOWARDS SUSTAINABILITY AND GREEN-AWARENESS". A & C, SUBMITTED TO "VSI: HPC IN COSMOLOGY AND ASTROPHYSICS" SPECIAL ISSUE"
- EUCLID COLLABORATION: P. MONACO, G. PARIMBELLI, M. Y. ELKHASHAB, J. SALVALAGGIO, T. CASTRO, M. D. LEPINZAN ET AL. (2025), "EUCLID PREPARATION. SIMULATING THOUSANDS OF EUCLID SPECTROSCOPIC SKIES", A & A, ACCEPTED FOR PUBLICATION ([ARXIV:2507.12116](https://arxiv.org/abs/2507.12116))
- EUCLID COLLABORATION: E. ROMELLI,....., M. D. LEPINZAN ET AL. (2025), "EUCLID QUICK DATA RELEASE (Q1): FROM IMAGES TO MULTIWAVELENGTH CATALOGUES: THE EUCLID MERGE PROCESSING FUNCTION", A & A, ACCEPTED FOR PUBLICATION ([ARXIV:2503.15305](https://arxiv.org/abs/2503.15305))

Candidate presentation

Candidate: Luca Cappelli

Cycle: XXXVIII

Supervisor: Giuseppe Murante

Co-supervisor: Stefano Borgani

Research Title: Quantum Algorithms for Cosmological Simulations

The Candidate has successfully accomplished the required educational activities as approved by the Teachers Board, including the Ph.D. courses, exams and the attendance of schools and conferences.

Brief description of the candidate research activity

Luca Cappelli's research has been dedicated to pioneering the application of Quantum Computing (QC) techniques to address fundamental and computationally demanding problems in astrophysics and cosmology, thereby establishing new theoretical and numerical frameworks for future-generation simulations and data analysis.

Quantum Computing is still a novel field, as far as its usage in the context of numerical extragalactic astrophysics is concerned. While QC is very well suited for solving linear problems, its application to nonlinear ones is still a vastly unsolved issue

One of Luca's main efforts involved the development of a novel quantum algorithm for the simulation of the gravitational evolution of cosmic density perturbations dominated by collisionless, non-baryonic Dark Matter (DM). This was achieved by introducing a method based on Variational Time Evolution (VTE) to simulate the non-linear Schrödinger-Poisson (SP) equation, which serves as a quantum-mechanical equivalent to the classical Vlasov-Poisson (VP) equation used in cosmological simulations. In fact, it can be shown that SP equations become the VP equations in the limit of the quantum coupling tending to zero. This approach is motivated by the potential for an exponential advantage in computational memory, allowing the encoding of N grid points into just $\log_2(N)$ qubits. Furthermore, his work rigorously addressed the numerical challenges and limitations of this quantum approach as it transitions towards the classical regime, specifically by examining the behavior of spatial resolution when the quantum coupling approaches zero. The results of this work have been presented in a research article, led by Luca, that has been already published

Complementary to his quantum focus, Luca's work also included a critical analysis of the classical numerical limits in integrating the VP equation, particularly for the stiff initial conditions of Cold Dark Matter (CDM), providing essential numerical insights into the suitability of different integration methods. Luca also performed a detailed comparison between SP equations, VP ones, and Particle-Mesh (PM) integration of cold non-collisional self-gravitating matter. His work shows the limits within which the integration of SP

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equations, also using a QC approach, can be used for simulating generic Cold DM dynamical evolution. Luca also investigated the problems in extending the VTE methods to 2D and 3D. The results obtained from this project are included in another paper, also led by Luca, which has been submitted for publication.

Furthermore, the candidate has also focused on computational optimization, proposing a quantum algorithm for the Fixed-Radius Neighbor Search (QFRANS) problem. This search is a critical and computationally intensive bottleneck in N-body simulations and data processing, where cache misses significantly slow down classical machines. The QFRANS algorithm, which leverages the fixed-point version of Grover's algorithm, is specifically designed to overcome these classical limitations by exploiting quantum parallelism. The development of this research is also presented in a research article, which has been submitted for publication.

Role of the Candidate and main achievements.

Luca Cappelli has demonstrated exceptional autonomy, technical skill, and leadership, successfully conducting state-of-the-art research at the critical intersection of quantum computing and cosmology. He has independently developed and analyzed complex quantum algorithms with high relevance for large-scale astrophysical simulations. Even if his Ph.D. project has been planned and closely followed by his supervisors, we should note that the technical Quantum Circuit programming work have been entirely done by him.

He conducted in full autonomy the complex development of the hybrid VTE algorithm for SP simulations, designed the innovative QFRANS algorithm, and performed the detailed numerical analysis of the classical VP equation. This body of work has yielded several refereed publications where he is the leading or first author (see the section on Publications). Overall, his work is highly innovative, directly addressing key computational bottlenecks in cosmology by proposing pioneering quantum solutions for simulation, data analysis, and optimization.

Luca had full responsibility for the preparation of the results for publication, also including paper writing, discussing with co-authors, interacting with the editor and referees. He was also very independent in the preparation of presentations for conferences, seminars and other meetings he has attended.

Luca was also very active in the PNRR Spoke-3 environment of the “National Center for HPC”, which focused on QC in Astrophysics. He participated at several discussions and workshops, and this brought to joint publications within the Spoke-3.

General evaluation of the candidate by the supervisor:

In summary, the Candidate has fully achieved the scientific targets set at the beginning of his Ph.D. program. Luca Cappelli is a highly proficient and independent researcher who has successfully bridged the gap between theoretical quantum computing and practical computational astrophysics. He has demonstrated a deep understanding of both the complexities of classical numerical methods and the potential (and limitations) of emerging

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quantum technologies. His ability to produce high-impact, first-author publications on sophisticated and timely subjects, coupled with his international collaborations (e.g., IBM Research), confirms his status as an excellent scientist ready to tackle the future challenges of large-scale computational science.

Luca was particularly able to develop and apply his QC programming skills to the problems tackled during his PhD and to discuss and share his skills with other members of the PNRR Spoke-3 initiative. Luca's work was always conducted in an independent, intuitive and careful way.

Overall, he showed motivation and determination in successfully working on his PhD project. He produced a significant amount of interesting and timely research work and acquired the fundamental skills of a researcher.

Summary:

In summary, the Teachers Board agrees that the candidate fully achieved the training and scientific targets set at the beginning of his Ph.D. program.

Presentations to Conferences, workshops, and meetings

- 1) INAF USC VIII meeting, 15-16 June 2023, Catania, contributed talk
- 2) Hydrosim Meeting, 17-21 July 2023, Sestri Levante, contributed talk
- 3) Quantum Computing and Simulation Workshop, 11-13 October 2023, Venice, poster
- 4) INAF SPOKE 10 Meeting, 21-22 November 2023, Bologna, presentation
- 5) Presentation at LRZ Garching, 6 March 2024, presentation
- 6) INAF SPOKE 10 Meeting, 15-18 April 2024 Napoli, presentation
- 7) Workshop on Quantum Simulation for fluid dynamics and cosmology, 22-29 July 2024, IFPU, presentation
- 8) INAF SPOKE 10 Meeting, 11-15 November 2024, Bologna, presentation
- 9) Winter School on Quantum Machine Learning, 9-13 December 2024, Trento, poster
- 10) PDP conference, 11-15 March 2025, Turin, contributed talk
- 11) Hydrosim meeting 28-31 July 2025, Trieste (07/2025), contributed talk

Publications

- “From Vlasov-Poisson to Schrödinger-Poisson: Dark matter simulation with a quantum variational time evolution algorithm”, L. Cappelli, F. Tacchino, G. Murante, S. Borgani, I. Tavernelli, Physical Review Research 6, 013282 (2024)
- “Quantum Algorithm for the Fixed-Radius Neighbor Search”, L. Cappelli, C. Sanavio, S. Succi, A.A. Zecchi, G. Murante, arXiv:2507.03445 (2025)
- “Numerical limits in the integration of Vlasov-Poisson equation for Cold Dark Matter”, L. Cappelli, G. Murante, S. Borgani, et al., arXiv:2503.22842 (2025)
- “The Application of Quantum Fourier Transform in Cosmic Microwave Background Data Analysis”, F. Farsian, A. Bulgarelli, M. Meneghetti, G. Sarracino, T. Trombetti, C. Burigana, V. Cardone, G. Murante, F. Schilliró, L. Cappelli, arXiv:2505.00650 (2025)

Candidate presentation

Candidate: Marco Dirindin

Cycle: XXXVIII

Supervisor: Daniele Coslovich

Co-supervisor: Maria Peressi

Research Title: Simulations of two-dimensional crystalline and amorphous oxides

The Candidate has successfully accomplished the required educational activities as approved by the Teachers Board, including the Ph.D. courses, exams and the attendance of schools and conferences.

Brief description of the candidate research activity

The candidate investigated the physical properties of two-dimensional (2D) oxides using large-scale molecular dynamics simulations and ab-initio methods. His PhD project involved two main research directions. First, starting from experimental data, he developed an effective classical potential to simulate the silica (SiO₂) bilayer as a strictly two-dimensional system. He used this potential to investigate the structure and dynamics of the amorphous 2D silica at low temperatures, testing several theoretical scenarios for the glass transition in network-forming glasses. A highlight of this work is the observation of large transient crystalline domains within the thermodynamically stable low-temperature liquid. These results point to a profound difference between glassy structure in two and three dimensions. As a second main project, he performed a systematic search for the crystalline polymorphs of the boria (B₂O₃) monolayer. He devised an algorithm to predict from first principles the structure of a boron-oxygen crystal experimental sample, recently synthesized at the CNR-Istituto Officina dei Materiali (IOM) laboratory in Basovizza (Trieste) by Alessandro Sala, Teresa Zio and collaborators. This work culminated in a joint publication in Science. After characterizing the crystalline monolayer, the candidate focused on the structure of amorphous experimental samples and developed an algorithm to recover the atomic positions from the experimental images, establishing contacts between the analysis of the silica bilayer and the boria monolayer. Overall, the work by the candidate shows that 2D oxides are an ideal test bench to assess theoretical scenarios for 2D melting and the glass transition in experiments.

Role of the Candidate and main achievements.

The candidate conceived, performed and analyzed all the simulations. He demonstrated a remarkable autonomy in performing all these tasks and required minimal guidance from the supervisor and co-supervisor. During his PhD project, he developed a range of computational tools to analyze simulation and experimental data. Two highlights are (i) an open source, well-documented library for the analysis of network structures and (ii) an efficient segmentation algorithm to analyze experimental STM images. He became knowledgeable with both molecular dynamics codes running on GPUs and Quantum

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ESPRESSO on hybrid CPU-GPU supercomputers. At the scientific level, his work led to a deeper understanding of 2D materials, both in their crystalline and amorphous forms. In addition to the publications indicated below, two other articles based on his PhD project's results are in preparation.

General evaluation of the candidate by the supervisor:

The candidate performed an excellent research work throughout his PhD project. He demonstrated a remarkable ability to coordinate and carry out complex research tasks, often involving the collaboration with experimentalists. He could solve physical problems autonomously, requiring minimal guidance from his supervisors. During the PhD project, he also significantly improved his presentation skills: his oral contribution at the EMRS 2025 Fall Meeting received an award for the best PhD student presentation. His technical writing skills in English are good. The candidate also actively co-supervised one MSc thesis and one Bachelor thesis in Physics. In conclusion, the candidate shows a strong potential for carrying out outstanding research work at the postdoc level.

Summary: The Teachers Board agrees that the candidate fully achieved the training and scientific targets set at the beginning of the Ph.D. program

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Presentations to Conferences, workshops, and meetings

Contributed talks:

- *Glassy dynamics and local crystalline order in two-dimensional amorphous silica*, NOMATEN Centre of Excellence, (Warsaw, Poland), September 19, 2025
- *From single bond to line defects: a case study from a novel two-dimensional network-forming material*, E-MRS 2025 Fall Meeting, University of Technology in Warsaw (Poland), September 18, 2025; the talk received the “Best PhD student presentation award”, funded by Elsevier
- *Glassy dynamics and local crystalline order in two-dimensional amorphous silica*, 10th International Discussion Meeting on Relaxations in Complex Systems (10 IDMRCS), (Barcelona, Spain), July 24, 2025
- *From single bond to line defects: a case study from a novel two-dimensional network-forming material*, Young Researchers’ Meeting of the European Theoretical Spectroscopy Facility (ETSF YRM 2025), SISSA (Trieste, Italy), May 26, 2025

Seminars:

- *Are glasses different in Flatland? Insights from a model of 2d amorphous silica*, Miramare campus, Department of Physics (Trieste, Italy), January 29, 2025

Posters:

- *Exploring two-dimensional crystalline phases of boron oxide on Pt(111)*, 22nd International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, International Center for Theoretical Physics (Trieste, Italy), January 08-10, 2025
- *Structure and dynamics of two-dimensional network-forming materials*, Liquid Matter Conference 2024, Mainz (Germany), September 22-27, 2024
- *Structure and dynamics of two-dimensional network-forming materials*, Course Topology and Materials at the International School of Physics “Enrico Fermi”, Varenna (Italy), July 17-22, 2024
- *Exploring a stochastic cost function landscape: the case of 2d amorphous silica*, Deep Modeling for Molecular Simulation 2023 school, Princeton University (United States of America), July 11-14, 2023

Publications

- T. Zio, M. Dirindin, C. Di Giorgio, M. Thaler, B. Achatz, C. Cepek, I. Cojocariu, M. Jugovac, T. O. Mente, A. Locatelli, L. L. Patera, A. Sala, G. Comelli, M. Peressi, C. Africh, *Two-dimensional diboron trioxide crystal composed by boroxol groups*, *Science*, 390(6768), 95-99 (2025) (DOI: <https://doi.org/10.1126/science.adv2582>)
- M. Dirindin, D. Coslovich, *Glassy dynamics and local crystalline order in two-dimensional amorphous silica*, *J. Phys. Chem. B*, 129, 3, 1095–1108 (2025) (DOI: <https://doi.org/10.1021/acs.jpcb.4c06881>)
- L. Figurato, M. Dirindin, J. L. Gaona-Reyes, M. Carlesso, A. Bassi, S. Donadi, *On the effectiveness of the collapse in the Di'osi–Penrose model*, *New Journal of Physics*, 26(11), 113004 (2024) (DOI: <https://doi.org/10.1088/1367-2630/ad8c77>)