SEDUTA DEL COLLEGIO DEI DOCENTI DEL 38° CICLO

06 Maggio 2026

Il Collegio dei Docenti del 38° ciclo del Dottorato di Ricerca in Scienze Fisiche e Chimiche dell'Università di Palermo, regolarmente convocato dal Coordinatore Prof. Marco Cannas, si riunisce alle ore 14,30 del giorno 16.12.2025 con il seguente ordine del giorno:

1) **Adempimenti per l'esame finale di conseguimento del titolo di dottore di ricerca del 38° ciclo (III° sessione)**

Presiede il Coordinatore Prof. Marco Cannas, svolge le funzioni di segretario il Prof. Simonpietro Agnello

Sono presenti

Marco Cannas, Francesco Ferrante, Simonpietro Agnello, Umberto De Giovannini, Alberto Pettignano, Gioacchino Massimo Palma, Francesco Ciccarello, Salvatore Lorenzo, Francesco Giannici, Giuseppe Lazzara, Giuseppe Cavallaro, Giovanni Marsella, Davide Valenti

Sono assenti giustificati Gianpiero Buscarino, Angelo Carollo, Tiziana Di Salvo, Claudio Fazio, Rosario Iaria, Stefana Milioto, Fabrizio Messina, Salvatore Miccichè, Marco Miceli, Roberto Passante, Lucia Rizzuto, Melania Del Santo, Giuseppina Micela.

Sono inoltre presenti i Dott. Lorenzo Lisuzzo, Angela Ciaravella, Manuela Mallamaci in qualità di cotutor.

Il Presidente, prof. M. Cannas, verificato il numero legale, dichiara aperta la seduta e passa a discutere il primo punto all'ordine del giorno:

1) Adempimenti per l'esame finale di conseguimento del titolo di dottore di ricerca del 38° ciclo (III° sessione)

Il presidente illustra gli adempimenti necessari per il conseguimento del titolo di dottore di ricerca per gli allievi del 38° ciclo che intendono sostenere l'esame finale nella terza sessione (26 Giugno – 06 Luglio 2026).

In accordo al cronoprogramma. il presente collegio dei docenti dovrà occuparsi dei seguenti punti:

- formulazione della relazione del dottorando sulle attività svolte

- formulazione del parere per il titolo di Doctor Europaeus

- proposta di formazione delle commissioni giudicatrici

- nomina dei valutatori esterni

Guercio Ludovico

(Tutor: Prof. Francesco Ferrante; Co-Tutor: Dott. Lorenzo Lisuzzo)

Il collegio prende visione della relazione dell'allievo (**allegato 1 al verbale**).

Il collegio propone che la commissione giudicatrice per l'esame finale sia composta da:

Membri effettivi

1) Prof. Giuseppe Domenico Arrabito, Università degli Studi di Palermo, giusppedomenico.arrabito@unipa.it

2) Prof. Carlo Adamo, Institute of Chemistry for Life and Health Sciences UMR CNRS 8060 - ENSCP Chimie Paris Tech - Parigi (Francia)

3) Prof. César Antonio Viseras Iborra, Department of Pharmacy and Pharmaceutical Technology Facultad de Farmacia - Universidad de Granada - Granada (Spagna)

Membri supplenti

Prof. Fabrizio Lo Celso, Università degli Studi di Palermo

Il collegio nomina i valutatori esterni:

1) Dmitry Yu Murzin, Åbo Akademi University, Turku, Finlandia

email: dmitry.murzin@abo.fi

2) Rawil Fakhrullin Kazan Federal University, Kazan, Russia

email: kazanbio@gmail.com

Inoltre, per l'allievo Guercio Ludovico, il collegio attesta che sono soddisfatti i criteri per conseguire il titolo di **Doctor Europaeus**, ed **esprime un parere positivo.**

Sangiorgi Emanuele

(Tutor: Prof. Simonpietro Agnello, Cotutor: Dott. Antonino Madonnia)

Il collegio prende visione della relazione dell'allievo (**allegato 2 al verbale**).

Il collegio propone che la commissione giudicatrice sia composta da:

Membri effettivi

1) Prof. Fabrizio Messina, Università degli Studi di Palermo, email: fabrizio.messina@unipa.it

2) **Prof. Luca Perfetti**, Ecole Polytechnique, Palaiseau (France)

3) Prof. Antonio Di Bartolomeo, Universita' Di Salerno (Italia)

Membri supplenti

Dott.ssa Alice Sciortino, Università degli Studi di Palermo

Prof. Emanuele Marino, Università degli Studi di Palermo

Il collegio nomina i valutatori esterni:

1) Yvon Cordier, Centre de Recherche sur l'Hétéro-Epitaxie et ses Applications, CNRS-CRHEA, Nice (France)

email: Yvon.Cordier@crhea.cnrs.fr

2) Martin Kalbac, J. Heyrovský Institute of Physical Chemistry, Prague (Czech Republic)

email: martin.kalbac@jh-inst.cas.cz

Inoltre, per l'allievo Sangiorgi Emanuele, il collegio attesta che sono soddisfatti i criteri per conseguire il titolo di **Doctor Europaeus**, ed **esprime un parere positivo.**

Cicciari Gloria Maria

(Tutor: Prof. Giovanni Marsella, Cotutor: Dott.ssa Manuela Mallamaci)

Il collegio prende visione della relazione dell'allieva (**allegato 3 al verbale**).

Il collegio propone che la commissione giudicatrice sia composta da:

Membri effettivi

1) Prof. Salvatore Micciche, Università degli Studi di Palermo, salvatore.micciche@unipa.it

2) Prof. Julian Rautenberg, Bergische Universität Wuppertal, Germany

3) Prof. Lorenzo Perrone, Università del Salento

Membri supplenti

Prof. Simonpietro Agnello, Università degli Studi di Palermo

Il collegio nomina i valutatori esterni:

1) Alvarez-Muniz Jaime, Universidad De Santiago De Compostela, Spain

email: jaime.alvarez@usc.es

2) Roth Markus, Karlsruhe Institute of Technology, Germany.

email: markus.roth@kit.edu

Inoltre, per l'allieva Cicciari Gloria Maria, il collegio attesta che sono soddisfatti i criteri per conseguire il titolo di **Doctor Europaeus**, ed **esprime un parere positivo.**

Pinto Marcel Augusto
(Tutor: Prof. Francesco Ciccarello)

Il collegio prende visione della relazione dell'allieva (**allegato 4 al verbale**).

Il collegio propone che la commissione giudicatrice sia composta da:
Membri effettivi
1) Prof. Angelo Carollo, Università degli Studi di Palermo, angelo.carollo@unipa.it
2) Dr. Simone Felicetti, Istituto CNR dei Sistemi Complessi, Roma
3) Prof. Fabrizio Illuminati, Università degli Studi di Salerno e Istituto CNR di Nanotecnologia

Membri supplenti
Prof. Salvatore Lorenzo, Università degli Studi di Palermo
Prof. Marco Di Liberto, Università degli Studi di Padova

Il collegio nomina i valutatori esterni:
1) Giuseppe Calajò, Università degli Studi di Padova
email giuseppe.calajo@unipd.it

2) Luca Chirolli, Istituto CNR dei Sistemi Complessi, Firenze
email: luca.chirolli@unifi.it

Aslam Rashida (Tutor: Prof. Massimo Palma, Cotutor: Dott.ssa Angela Ciaravella)

Il collegio prende visione della relazione dell'allieva (**allegato 5 al verbale**).

Il collegio propone che la commissione giudicatrice sia composta da:

Membri effettivi

1) Dott. Giacomo Mulas, INAF – Osservatorio Astronomico di Cagliari

2) Prof. Marco Miceli, Università degli Studi di Palermo, marco.miceli@unipa.it

3) Prof. Apollaro Tony John George, L-Università ta' Malta (UM)

Membri supplenti

Prof. Francesco Ciccarello, Università degli Studi di Palermo

Il collegio nomina i valutatori esterni:

1) Guillermo Munoz-Caro, Departamento de Astrofísica – Centro de Astrobiologia, Torrejón de Ardoz (Madrid)

email: munozcg@cab.inta-csic.es

2) Yu-Jung Chen, Physics Department, National Central University, Jhongli City - Taiwan

email: asperchen@phy.ncu.edu.tw

Vetrano Marco
(Tutor: Prof. Massimo Palma, Cotutor: Prof. Salvatore Lorenzo)

Il collegio prende visione della relazione dell'allieva (**allegato 6 al verbale**).

Il collegio propone che la commissione giudicatrice sia composta da:
Membri effettivi
1) Dott. Giacomo Mulas, INAF – Osservatorio Astronomico di Cagliari
2) Prof. Marco Miceli, Università degli Studi di Palermo, marco.miceli@unipa.it
3) Prof. Apollaro Tony John George, L-Università ta' Malta (UM)

Membri supplenti
Prof. Francesco Ciccarello, Università degli Studi di Palermo

Il collegio nomina i valutatori esterni:

1) Francesco Plastina, Università della Calabria
email: francesco.plastina@fis.unical.it

2) Giuseppe Germano Sacco, INAF-Osservatorio Astrofisico di Arcetri
email: germano.sacco@inaf.it

Il verbale è approvato seduta stante. La seduta si chiude alle ore 15:00.

Il Presidente
Prof. Marco Cannas

Il Segretario
Prof. Simonpietro Agnello

Allegato 1

PHD IN PHYSICAL AND CHEMICAL SCIENCES, XXXVIII COURSE

PhD Candidate: Ludovico Guercio

Transcript of Records

Tutor: Prof. Francesco Ferrante

Cotutor: Dott. Lorenzo Lisuzzo

Courses/school/exam scores:

- Advanced microscopy and spectroscopy techniques applied to nanomaterials", S. Agnello e G. Buscarino, University of Palermo. Exam taken.
- "Introduction to DFT and TDDFT", U. De Giovannini, University of Palermo. Exam taken.
- "Organic/inorganic nanocomposites: thermodynamics, structure and applications", G. Cavallaro, University of Palermo. Exam taken.

- "SEM training: potenzialità e utilizzo della microscopia elettronica a scansione (SEM)", G. Nasillo, University of Palermo
- "SMART-X Workshop on X-ray Spectroscopy and Related Phenomena", University of Palermo
- "Normal Dynamics: solving Newton's equations of motion in the reciprocal space", A. Cammarata, University Palermo.
- "Towards a universal framework to describe and control atom-scale friction", A. Cammarata, University of Palermo.
- "ILL Soft Matter Summer School", Grenoble.

Research and training periods abroad

6 months Research period at the University of Malaga, Spain, from october, 4th 2024 to april, 4th 2025. Scientific research about the conversion of furfural to valuable compounds by means of saponite clay catalysts. This activity was inherent to the PhD project.

Papers published:

Related to the PhD project

1. Guercio, L.; Ferrante, F.; Bertini, M.; Ferlito, C.; Duca, D.
DFT investigation of gold clusters growth on bifunctionalized halloysite surface
In preparation

2. Guercio, L.; Ferlito, C.; D'Agostino, G.; Cavallaro, G.; Lazzara, G.; Dolgan, K.
Hierarchical Oil–Water–Oil Pickering Double Emulsions Stabilized by Tubular Nanoparticles.
Journal of the American Chemical Society, in press
https://doi.org/10.1021/jacs.6c01861

3. Guercio, L.; Ferrante, F.; Bertini, M.; Ferlito, C.; Lisuzzo, L.; Lazzara, G.; Duca, D.
Anchoring Gold Nanoparticles on Functionalized Halloysite Nanotubes: Density Functional Theory and Experimental Studies.
The Journal of Physical Chemistry C, 2025, 129, 16944.
https://doi.org/10.1021/acs.jpcc.5c05165

4. Guercio, L.; Ferrante, F.; Bertini, M.; Gueci, L.; Lisuzzo, L.; Duca, D.
Selecting the Most Suitable DFT Exchange–Correlation Functional for Consistent Modeling of Subnanometric Gold Clusters in Catalytic Systems.
Catalysts, 2025, 15, 1083.
https://doi.org/10.3390/catal15111083

5. Lisuzzo, L.; Guercio, L.; Cavallaro, G.; Lazzara, G.; Duca, D.; Ferrante, F.
Halloysite Clay Nanotubes for Catalytic Conversion of Biomass: Synergy between Computational Modeling and Experimental Studies.
ACS Catalysis, 2024, 14, 18167.
https://doi.org/10.1021/acscatal.4c05907

6. Bertini, M.; Ferrante, F.; Guercio, L.; Lisuzzo, L.; Duca, D.
Modified Halloysite as Catalyst for the Conversion of Hydroxymethylfurfural to Furandicarboxylic Acid: A DFT Investigation.
ChemCatChem, 2024, 16, e202400179
https://doi.org/10.1002/cctc.202400179

Other ISI papers:

7. Guercio, L.; Ferlito, C.; Cavallaro G.; Lazzara G.; Hueckel T.; Lisuzzo L.; Sacanna S.
Pickering-Engineered Microparticles for Magnetically Guided Motion and Light-Triggered Catalysis.
Submitted

8. Ferlito, C.; Ferrante, F.; Bertini, M.; Guercio, L.; Lazzara, G.; Duca, D.
Computational Study of the Early Stages of Ibuprofen Degradation on Manganese Dioxide
In preparation

Conferences/workshop attended:

Talks:

- *Halloysite based catalysts: computational and experimental investigations into biomass conversion*, Guercio L., Bertini M., Ferrante F., Lisuzzo L., Duca D. Expanding Clay Science: Over the Pacific and Beyond – 61st Annual Meeting of the Clay Minerals Society *(on line)*. 03/06/24 – 06/06/24
- *Toward Green Catalysis with Halloysite–Gold Nanocomposites Materials*, Guercio L., Ferrante F. Bertini M., Lisuzzo L., Ferlito C., Cavallaro G., Lazzara G., Duca D. International Clay Conference, Trinity College, Dublin. 13/07/25 – 19/07/25.

Posters:

- Halloysite based nanocatalysts for the catalytic conversion of biomass, Guercio L., Bertini M., Ferrante F., Lisuzzo L., Duca D. SciSiCa: Congresso congiunto delle sezioni Calabria e Sicilia. 11-12 Dicembre 2023
- *Halloysite based gold nanocatalysts for the catalytic conversion of biomass*, Guercio L. , Bertini M., Duca D., Ferrante F., Lazzara G., Lisuzzo L. PCCP 25th anniversary symposium, University of Amsterdam 01/05/24 – 02/05/24
- "Optimizing Pickering Emulsions with Surface-Modified Halloysite Nanotubes", Guercio L., Ferlito C., Ferrante F., Lisuzzo L., Lazzara, G. and Duca D., ILL Soft Matter Summer School, 30/06/25-03/07/25.

Thesis title:

Sustainable Clay Based Nanocomposites for Biomass Valorization

Abstract:

Within the broader context of sustainability, increasing attention has been directed toward addressing key challenges in contemporary environmental and chemical systems. In this perspective, particular emphasis is placed on the valorization of biomass-derived platform molecules and the development of sustainable catalytic and material-based approaches.

This study focuses on furfural and its key derivatives, especially 5-hydroxymethylfurfural (HMF) and 2,5-furandicarboxylic acid (FDCA), which represent central intermediates in the conversion of renewable resources into high-value chemicals. In parallel, natural clay minerals are investigated as versatile and sustainable supports for surface modification and functionalization, providing a green and abundant alternative to conventional catalytic or structural materials.

The research strategy integrates theoretical and experimental approaches. Density functional theory calculations are employed to gain molecular-level insight into the interactions governing the investigated systems, while experimental work includes the synthesis and characterization of functional materials and catalytic systems.

The results obtained provide a solid foundation for future investigations. In particular, a novel catalytic system potentially applicable to the conversion of HMF into FDCA was explored. In parallel, a system aimed at the valorization of furfural into high-value materials was investigated. Furthermore, the development of a dynamic oil-in-water-in-oil (O/W/O) Pickering emulsion system was achieved, with potential applications in catalysis and waste treatment processes.

Overall, this work contributes to the advancement of sustainable chemical strategies by combining biomass valorization, clay-based functional materials, and integrated theoretical–experimental methodologies.

The PhD Board Dean

Prof. Marco Cannas

Allegato 2

PHD IN PHYSICAL AND CHEMICAL SCIENCES, XXXVIII COURSE

PhD Candidate: Emanuele Sangiorgi

Transcript of Records

Tutor: Prof. Simonpietro Agnello

Cotutor: Dott. Antonino Madonia

Courses/school/exam scores:

- Project Management in The Scientific-Spatial Context (Prof.ssa Giuseppina Micela, 20 hours)
- Advanced microscopy and spectroscopy techniques applied to nanomaterials (Prof. S. Agnello, Prof. G. Buscarino, 20 hours)
- Organic/Inorganic Nanocomposites: thermodynamics, structure, and applications (Prof. G. Cavallaro, 20 hours)

Research and training periods abroad

- 04/04/2024 – 07/10/2024; Research period abroad under the supervision of Prof. Béla Pécz, Institute of Technical Physics and Materials Science, Budapest, Hungary.

Papers published:

1. **E. Sangiorgi**, A. Madonia, G. Laurella, S. E. Panasci, E. Schilirò, F. Giannazzo, I. Píš, F. Bondino, G. Z. Radnóczi, V. Kovács-Kis, B. Pécz, G. Buscarino, F. M. Gelardi, M. Cannas, and S. Agnello, "Mild Temperature Thermal Treatments of Gold-Exfoliated Monolayer MoS2, " *Nanomaterials*, vol. 15, no. 3, p. 160, Jan. 2025.

2. G. Puleo, M. Maggiore, E. Rosa, C. Pellerito, G. Cavallaro, P. G. Medaglia, **E. Sangiorgi**, P. Conti, S. A. Fortuna, V. Ferrara, S. Agnello, B. Pignataro, F. Campanile, and G. Arrabito, "Exploring ZnO microcrystals through experimental design: from solar photocatalysis to antibacterial activity," *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, p. 139958, Feb. 2026.

3. **E. Sangiorgi**, A. Madonia, F. Migliore, A. Alessi, R. Grasset, O. Cavani, S. E. Panasci, E. Schilirò, F. Giannazzo, F. Esposito, L. Seravalli, M. Cannas, and S. Agnello, "Irradiation-Resistant Heterostructures Based on Monolayer MoS2," *Physica status solidi (a)*, vol. 223, no. 6, p. e202500759, Mar. 2026.
4. **E. Sangiorgi**, F. Migliore, A. Madonia, S. E. Panasci, E. Schilirò, F. Giannazzo, F. Esposito, L. Seravalli, G. Buscarino, M. Cannas, and S. Agnello. "Role of Thermodynamic Variables on 2D Molybdenum Disulfide Thermal Treatments". *Il Nuovo Cimento (Accepted)*

Conferences/workshop attended:

Talks:

- "Strain-doping tailoring of MoS_2 on Au substrate under controlled environment conditions", September 2023, E-MRS 2023 Fall Meeting – *Warsaw, Poland*
- "Tunable physical properties of MoS_2 for optoelectronic devices: substrate interaction and strain-doping tailoring in thermally controlled conditions", May 2024, E-MRS 2024 Spring Meeting – *Strasbourg, France*
- "Tunable physical properties of MoS_2 for optoelectronic devices induced by strain via heat treatment", September 2024, E-MRS 2024 Fall Meeting – *Warsaw, Poland*
- "Post-synthesis modification of physical properties of 2D MoS_2 on an insulating substrate", June 2025, WOCSDICE - EXMATEC 2025 – *Cádiz, Spain*
- "Thermal modulation of optical and electronic features of 2D Molybdenum Disulfide on SiO_2/Si", September 2025, 111th National Congress of the Italian Physical Society – *Palermo, Italy*

Posters:

- "Tuning the luminescence and structural properties of single layer MoS_2 for optoelectronic devices under thermally controlled conditions" May 2024, E-MRS 2024 Spring Meeting – *Strasbourg, France*
- "MoS_2 Monolayer Physical Properties — Engineering in Temperature-Controlled Environments" December 2024, 2024 MRS Fall Meeting and Exhibit – *Boston, Massachusetts*
- "2D MoS_2 post-synthesis improvement of optical and electronics properties", October 2025, AFuN25 - International Summer School on Advanced Functional Nanomaterials – *Palermo, Italy*

Thesis title:

Electronic and Structural Modifications in 2D Semiconductors

Abstract:

The advent of two-dimensional (2D) Transition Metal Dichalcogenides (TMDCs), particularly molybdenum disulfide (MoS_2), has opened new frontiers in next-generation optoelectronics. At the monolayer limit, MoS_2 exhibits a direct bandgap and strong light-matter interactions. However, the intrinsic electronic and optical properties of 1L-MoS_2 are highly sensitive to the underlying environment and the fabrication process. Interfacial phenomena, such as mechanical strain and charge carrier injection (doping) induced by the substrate, often dictate the final device performance.
This thesis systematically investigates the interfacial interactions between monolayer MoS_2 and a diverse set of target substrates, encompassing metallic (Au), insulating (SiO_2), and semiconducting (GaN) platforms. To provide a comprehensive overview, the study compares samples obtained

through different fabrication regimes: top-down approaches, specifically Gold-Assisted Exfoliation (GAE) and Gold-Assisted Transfer (GAT), and bottom-up synthesis via Chemical Vapor Deposition (CVD). High-resolution spatial mapping via micro-Raman spectroscopy, Photoluminescence (PL), and Atomic Force Microscopy (AFM) was employed to decouple the effects of built-in strain and substrate-induced doping on the excitonic emission of the 2D layer.
The core objective of this work was to actively modify and enhance the post-synthesis properties of the MoS_2 layer. To achieve this, targeted thermal treatments were performed on the heterostructures. The results demonstrate that controlled annealing serves as a powerful tool to modulate the layer-substrate coupling. Thermal processing effectively redistributes interfacial strain, alters the local charge concentration, and passivates structural defects. Consequently, a significant modulation of the optical yield and excitonic recombination dynamics was observed.
Ultimately, this comparative study establishes a comprehensive framework for understanding how different substrates and post-synthesis thermal engineering dictate the physical state of 2D MoS_2. By successfully optimizing its electronic and optical properties, this thesis provides a reliable pathway for integrating monolayer MoS_2 into high-performance optoelectronic and photonic architectures.

The PhD Board Dean

Prof. Marco Cannas

Allegato 3

PHD IN PHYSICAL AND CHEMICAL SCIENCES, XXXVIII COURSE

PhD Candidate: Gloria Maria Cicciari

Transcript of Records

Tutor: Prof. Giovanni Marsella

Cotutor: Dott.ssa Manuela Mallamaci

Courses/school/exam scores:

- Experimental techniques in astroparticle physics (20 h) - Prof. G. Marsella;
- Millisecond Pulsars: Theory and Observations (20 h) - Prof. R. Iaria;
- Project Management in the Scientific-Spatial Context (20 h) - Dr.ssa G. Micela.

Research and training periods abroad

- LST-1, Roque de los Muchachos Observatory (ORM), La Palma - November 17th, 2024 - December 11th, 2024;
- Max Planck Institute for Physics, Garching - January 20th, 2025 - July 8th, 2025 - Supervisor: Dr. Alessio Berti
- Centre de Physique des Particules de Marseille (CPPM), Marseille - March 21th, 2026 - April 4th, 2026.

Papers published:

- Abe K., et al. (including Cicciari G. M.), "CTAO LST-1 observations of magnetar SGR 1935+2154: Deep limits on sub-second bursts and persistent tera-electronvolt emission", *Astronomy & Astrophysics*, 706, A25, 2026.
- Abe K., et al. (including Cicciari G. M.), "VHE γ-ray observations of bright BL Lacs with the Large-Sized Telescope prototype (LST-1) of the CTAO", *arXiv preprint arXiv:2510.03702*, 2025.
- Abe K., et al. (including Cicciari G. M.), "Constraining the TeV gamma-ray emission of SN 2024bch, a possible type IIn-L from a red supergiant progenitor", *Astronomy & Astrophysics*, 702, A125, 2025.
- Cicciari G. M., et al., "Investigating the capability of the Cherenkov Telescope Array Observatory to detect gamma-ray emission from simulated stationary neutrino sources identified by KM3NeT", *arXiv preprint arXiv:2509.12910*, 2025.
- Abe K., et al. (including Cicciari G. M.), "Detection of the Geminga pulsar at energies down to 20 GeV with the LST-1 of CTAO", *The Astrophysical Journal Letters*, 974 (2), L17, 2025.
- Abe K., et al. (including Cicciari G. M.), "A detailed study of the very-high-energy Crab pulsar emission with the LST-1", *Astronomy & Astrophysics*, 690, A293, 2025.

- Abe K., et al. (including Cicciari G. M.), "Detection of RS Oph with LST-1 and modelling of its HE/VHE gamma-ray emission", *Astronomy & Astrophysics*, 690, A30, 2024
- Abe K., et al. (including Cicciari G. M.), "Performance of the joint LST-1 and MAGIC observations", *Astronomy & Astrophysics*, 680, A66, 2023.

Proceedings of Science

- Cicciari, G. M., Ferrara G., Mallamaci M., Marsella G., Sergijenko, O., "Investigating Cherenkov Telescope Array Observatory capability to detect gamma-ray emission from simulated neutrino sources identified by KM3NeT", *39th ICRC*, PoS(ICRC2025)1015, 2026.
- Seglar Arroyo, M., A. Berti, A. Carosi, Cicciari G. M., et al., "Transient Observations with LST-1: Key Results and Future Prospects", *39th ICRC*, PoS(ICRC2025)1014, 2026.
- Mineo T., Mollica, D., Compagnino A. A., Cicciari G. M., et al., "Using muon rings for the optical calibration of ASTRI-1 telescope: preliminary results", *39th ICRC*, PoS(ICRC2025)761, 2026.
- Abe K., et al. (including Cicciari G. M.), "Observation of the Crab Pulsar with the LST-1", *38th ICRC*, PoS(ICRC2023)623, 2024.
- López-Oramas A., et al. (including Cicciari G. M.), "Search for VHE gamma-ray emission from the Binary System PSR B1259-63/LS 2883 with LST-1", *38th ICRC*, PoS(ICRC2023)644, 2024.
- Morcuende D., et al. (including Cicciari G. M.), "Observations of Galactic sources with LST-1: Geminga and the Galactic Center", *38th ICRC*, PoS(ICRC2023)715, 2024.
- Kobayashi Y., et al. (including Cicciari G. M.), "LST-1 observations of the recurrent nova RS Ophiuchi", *38th ICRC*, PoS(ICRC2023)664, 2024.

Conferences/workshop attended:

- Talks:

· CTAO Consortium meeting - Paris, April 13th 2026 - April 17th 2026;

· TeV Astrophysics Particle 2025 - Valencia, November 3rd 2025 - November 7th 2025;

· 111° Congresso Società Italiana di Fisica (SIF) - Palermo, September 22th 2025 - September 26th 2025

· CTA-KM3NeT community day - Amsterdam, September 8th 2025;

· 2nd VHEGAM meeting - Bari, May 26th 2025 - May 28th 2025;

· CTAO Consortium Science meeting - Garching, May 12th 2025 - May 16th 2025;

· CTA-SCT/CTA-US 2024 Winter Meeting - Tucson, January 20th, 2024 (online participation);

- CTAO Science Symposium 2024 - Bologna, April 15th, 2024 - April 18th, 2024;

- 1st VHEGAM meeting: LST-Italia proposals - Bologna, January 15th, 2024 - January 17th, 2024;
- Journal Club@IASF-PA - Palermo, November 7th, 2023;
- German-Italian Physics Exchange 2023 (GIPE23) - Bari, October 5th, 2023 - October 9th, 2023.

- Posters:

- ICRC 2025 - The Astroparticle Physics Conference - Geneva, July 14th 2025 - July 24th 2025;
- The Fifth Gravi-Gamma-Nu workshop - Bari, October 9th 2024 - October 11th 2024.

- Partecipations:

- Workshop on Numerical Multi Messenger Modeling - DESY, February 26th 2025 - February 28th 2025 (online participation).
- F2F MAGIC+LST Science Meeting - Garching, January 13th 2025 - January 17th 2025.
- LST General Meeting, Online, November 2024, Part 1 - November 11th 2024 - November 15th 2024 (online participation);
- The 13th IDPASC school - Palermo and Catania, September 17th 2024 - September 27th 2024;
- Fourth ML-INFN Hackathon: Starting Level - online, June 21th, 2024 - June 23th, 2024;
- 13th CRIS-MAC 2024 (Cosmic-Ray International Studies and Multi-messenger Astroparticle Conference) - Trapani, June 17th 2024 to June 21st 2024 (LOC member)
- LST General Meeting - Prague, May 20th 2024 - May 24th 2024 (online participation);
- CTAO/CTAC Science meeting - Bologna, April 18th, 2024 - April 19th, 2024;
- Workshop on Numerical Multi-messenger Modeling - online, February 21th, 2024 - February 23th,
- 2nd LST Analysis school, online - February 5th, 2024 - February 9th, 2024;
- The Horizon Europe framework program: opportunities to support young researchers and develop their early-stage careers, Palermo - February 5th 2024;
- AVENGe - Advances in Very-High Energy Astrophysics with Next-Generation Cherenkov Telescopes - Roma, May 29th, 2023 - May 31th, 2023.

Thesis title:

Perspectives in multi-messenger astronomy: real-time follow-up to unravel gamma-ray counterparts from neutrino alerts with Cherenkov Telescope Array Observatory

Abstract:

In this thesis, I analyze the prospects for multi-messenger astrophysics in the era of next-generation observatories, focusing in particular on the real-time identification of very high-energy (VHE) gamma-ray counterparts associated with astrophysical neutrino alerts. The detection of a common source for both messengers is a fundamental requirement for identifying the cosmic accelerators of VHE cosmic rays, which would otherwise be deflected by galactic and intergalactic magnetic fields.

A significant portion of this work is dedicated to evaluating the detection capabilities of the future Cherenkov Telescope Array Observatory (CTAO). Using the FIRESONG framework, I performed extensive simulations of extragalactic neutrino source populations, considering both steady-state emitters and transient sources with flares similar to the blazar TXS 0506+056. I then developed and applied a filtering pipeline dedicated to these populations, using the detection potential and effective area of current neutrino detectors to identify the most promising candidates for electromagnetic follow-up. To assess their detectability, I developed an original analysis chain, implementing the Gammapy framework for the first time to model the CTAO response and calculate the detection potential. Particular emphasis was placed on KM3NeT/ARCA; I demonstrated that its strategic location in the northern hemisphere provides an optimal view of the southern sky, offering a unique synergy with CTAO-South that effectively complements the coverage provided by IceCube.

As a crucial step toward operational readiness, I focused on the development and validation of the "Transient Handler" for the Large-Sized Telescope (LST-1), the precursor to CTAO-North. This system is designed to handle the reception of external alarms and trigger automatic telescope repositioning. I conducted a detailed analysis of the system's performance and latency, which are essential for capturing rapidly fading transient emissions.

Furthermore, I applied the multi-messenger analysis pipeline to real data collected by LST-1 during Target-of-Opportunity (ToO) campaigns. Specifically, I analyzed observations of potential neutrino sources, including the high-redshift blazar PKS 1424+240 and the BL Lac object VER J0521+211. Although no significant gamma-ray excess was detected during these periods, I derived rigorous 95% C.L. upper limits on the VHE flux. These results provide critical constraints on hadronic emission models and on the contribution of these sources to the diffuse neutrino flux during their quiescent states.

In conclusion, this thesis demonstrates that the combination of the CTAO's unprecedented sensitivity and low energy threshold (down to ~20 GeV) with optimized real-time follow-up strategies will be fundamental to the future of multi-messenger astronomy. The validated analysis pipelines and performance studies presented here lay the groundwork for the future discovery of the high-energy sources that power the non-thermal Universe.

The PhD Board Dean

Prof. Marco Cannas

Allegato 4

PHD IN PHYSICAL AND CHEMICAL SCIENCES, XXXVIII COURSE

PhD Candidate: Marcel Augusto Pinto

Transcript of Records

Tutor: Francesco Ciccarello

Cotutor:

Courses/school/exam scores:

Mandatory Training:

- I(TD)DFT - Prof. Umberto di Giovanini
- Quantum Optics & Topology in Photonic Lattices – Prof. Francesco Ciccarello and Prof. Angelo Carolo
- Open Quantum Systems and Quantum Machine Learning – Prof. Salvatore Lorenzo and Prof. Luca Innocenti

Schools:

- Winter School: *Tensor Network based approaches to Quantum Many-Body Systems.* University of Padova, Padova (Italy), 13-17 May (2024)
- Summer School: *Generation QI, Picturing Quantum Weirdness.* University of Gdansk, Gdansk (Poland), 7-19 August (2023) – Online
- Summer School: *Generation QI, Quantum Cryptography.* University of Gdansk, Gdansk (Poland), 17-28 July (2023)

Research and training periods abroad

- 01/05/2025 – 30/10/2025: Research period at Consejo Superior de Investigaciones Cientificas (CSIC), Madrid, Spain. Tutor: Prof. Alejandro Gonzáles Tudela

Papers published:

1. **M. A. Pinto**, G. L. Sferazza, D. Di Bernardis & F. Ciccarello. *Non-Markovian dynamics of a qubit due to accelerated light in a lattice.* Phys. Scr. 100 105304 (2025)

Papers submitted or in preparation:

1. E. Di Benedetto, X. Sun, **M. A. Pinto**, L. Leonfore, C. Chang, V. Jouanny, L. Peyruchat, P. Scarlino & F. Ciccarello. *Emergent cavity-QED dynamics along the edge of a photonic lattice* arXiv:2507.13444 (2025) (Submitted)
2. **M.A. Pinto**, G. L. Sferazza, S. Casulleras, D. Di Bernardis, A. Gonzáles-Tudela & F. Ciccarello. *Giant-Atom Valleytronics: Selective Coupling and Chiral Photon Emission.* (2026) (In preparation)
3. J. T. Schneider, **M. A. Pinto**, C. Tabares, A. Muñoz de las Heras & A. González-Tudela. *Scalable spin squeezing in a WQED platform* (2026) (In preparation)

Conferences/workshop attended:

- Talks:
  - **M. A. Pinto**, G. L. Sferrazza, D. Di Bernardis & F. Ciccarello. *Emission of (Giant) atoms under an electric field.* Secondo Congresso Nazionale NQSTI, Rome, Italy (2025)
  - **M. A. Pinto**, G. L. Sferazza, D. Di Bernardis & F. Ciccarello. *Emission of (Giant) atoms under an electric field.* Quantum Technologies for Young Researchers workshop (QTYR25), Madrid, Spain (2025)
- Posters:
  - **M. A. Pinto**, G. L. Sferrazza & F. Ciccarello. *Chiral emission of giant atoms in 2D.* IQIS 2023 Italian Quantum Information Science, Trieste, Italy (2023)
  - **M. A. Pinto**, G. L. Sferazza, D. Di Bernardis & F. Ciccarello. *Chiral emission mediated by a giant atom in a honeycomb photonic bath.* QSG 2024 Quantum Science Generation, Trento, Italy (2024)
  - **M. A. Pinto**, G. L. Sferrazza, D. Di Bernardis & F. Ciccarello. *Non-Markovian dynamics of a qubit due to accelerated light in a lattice.* WQED 2025 Waveguide Quantum Electrodynamics, Erice, Italy (2025)
  - **M. A. Pinto**, G. L. Sferrazza, D. Di Bernardis & F. Ciccarello. *Non-Markovian dynamics of a qubit due to accelerated light in a lattice.* IQIS 2025 Italian Quantum Information Science, Bologna, Italy (2025)
  - **M. A. Pinto**, G. L. Sferazza, D. Di Bernardis & F. Ciccarello. *Non-Markovian dynamics of a qubit due to accelerated light in a lattice.* Progress in Photonic Quantum Computing, Bad Honnef, Germany (2025)

Academic Service Activities:

- **Conferences organization:**
  - Local Organizer at **WQED 2025 Waveguide Quantum Electrodynamics**, Erice, Italy (2025), Website: https://wqed25.weebly.com/
  - Local Organizer at **WQED 2023 Waveguide Quantum Electrodynamics**, Erice, Italy (2023), Website: https://wqed23.weebly.com
- **Local organization:**
  - Organization of the weekly group seminar at the **Quantum Unipa group (QUniPa).** Website: https://quantum.unipa.it/

Thesis title: Emission Dynamics of a Qubit in Photonic Lattices with Synthetic Potentials

Abstract:

Engineering the on-site frequencies of a photonic lattice provides a powerful route to endow emitted photons with non-trivial dynamical and topological properties, reshaping the way a coupled qubit decays. This thesis investigates the emission dynamics of a qubit weakly coupled to photonic lattices hosting such synthetic potentials, showing how the resulting band structure dictates qualitatively distinct regimes of light-matter interaction.

In the first part, we study a qubit coupled to a one-dimensional coupled-cavity array with a linear gradient in the cavity frequencies, which acts on photons as a synthetic force F. For strong F, emission becomes reversible and is captured by an effective Jaynes-Cummings model, producing a chiral, time-periodic excitation of an extended region of the array, either to the right or to the left of the qubit depending on its frequency. For weak F, the decay is non-Markovian and exhibits revivals reminiscent of atoms between mirrors, even though no mirrors are present: the finite bandwidth confines the emitted photon, and the dynamics is well described by a delay differential equation in which the amplitude and period of Bloch oscillations play the role of cavity length and round-trip time.

In the second part, we move to two dimensions and couple a *giant atom*, a qubit with multiple, spatially separated coupling points, non-locally to a honeycomb lattice of resonators with detuned sublattice frequencies. By suitably arranging the coupling points, the giant atom selectively addresses a single valley, a capability unattainable with a local emitter. This valley-selective coupling endows the emitted photons with an effective valley-polarized Berry curvature, giving rise to valley-polarized edge modes at domain walls between regions of opposite sublattice detuning. As a consequence, a giant atom placed near such a domain wall exhibits chiral emission of valley-polarized photons without breaking time-reversal symmetry, suggesting a natural implementation in circuit QED.

Together, these results establish synthetic potentials in photonic lattices as a versatile tool for controlling qubit emission, linking waveguide QED to Bloch-oscillation physics and to valleytronics.

The PhD Board Dean

Prof. Marco Cannas

Marco Cannas

Allegato 5

PHD IN PHYSICAL AND CHEMICAL SCIENCES, XXXVIII COURSE

PhD Candidate:.Rashida Aslam.

Transcript of Records

Tutor: Prof. Gioacchino Massimo Palma

Cotutor: Angela Ciaravella

Courses/school/exam scores:

- **Astrochemistry.** Mode of attendance is in person (By Cesare Cecchi Pestellini, at INAF, Palermo)
- **Design and Development of Bioactive Molecules.** Mode of attendance is in person (Prof. Marco Tutone, Prof. Maria Valeria Raimondi , Department of Biological, Chemical and Pharmaceutical Sciences and Technologies (STEBICEF) , UNIPA). Total 16 lectures, (32 hours)
- **Magnetohydrodynamics in astrophysical context.** Mode of attendance is in person (INAF, Palermo). Total 6 lectures, (20 hours)
- **Soft Matter** Mode of attendance is in person (by Prof. Thomas E. Kodger at department of Physical and chemical sciences, UNIPA, Palermo). Total 6 lectures, (18 hours)
- **Astrochemistry-From the Big bang to Life.** Mode of attendance is online (Heriot-Watt University, Scotland). Total 18 lectures, (36 hours)
- **Fundamentals of data management plan and data models in Astrophysics**. Mode of attendance is online (24 to 25 January, 2024, Basevi Castle - INAF Astronomical Observatory of Trieste).
- **Attended International Astrobiology School for 4 days** (Florence, Italy)

Research and training periods abroad.

6 months at National Central University (NCU), Taoyuan, Taiwan.

Papers published: 0

Paper Accepted: AAS73569R2

Title: CO LINE PROFILES IN ACCRETING ICES
In Astrophysical Journal (APJ)

Paper in Process:

Title: Beyond habitability: a computational data mining approach extremophiles based" (in preparation and at an advanced stage); it will be submitted to "International Journal of Astrobiology"

Conferences/workshop attended:

Attended the conference entitled "Workshop on Interstellar Matter (ISM) 2025" held November 12 to 14, 2025 at Naoki Watanabe Institute of Low Temperature Science Hokkaido University, Japan

Posters:

CO Infrared Band Profiles as a Probes of Interstellar Ice Condensation

Thesis title:

"Radiation and Surface-Driven Evolution of Prebiotic Astrophysical Ice"

Abstract:

The evolution of chemical complexity in the Universe is a fundamental journey bridging the cold, vast expanse of interstellar and circumstellar space with the emergence of planetary bodies and the potential for life. This thesis investigates the physical and chemical transformation of icy dust grain mantles, specifically focusing on the internal architecture of these condensates as they form on mineral dust backbones. A central objective of this work is to determine whether these mantles form homogeneously mixed chemical environments or organize into distinct, segregated domains. Distinguishing between these two structural architectures is crucial, as the specific molecular "neighborhood" in which a species resides directly constraint the reaction pathways available during energetic processing. Consequently, the physical arrangement of the ice, whether layered or mixed, ultimately shapes the molecular complexity available for prebiotic chemistry.

To bridge laboratory simulations with the physical reality of the interstellar medium (ISM), we utilize a deposition protocol that serves as a structural proxy for astrophysical processes. While species like water do not exist in high gas-phase abundance in the ISM, they form directly on grain surfaces through the hydrogenation of precursors. Because atomic hydrogen is highly mobile even at T~10 K, leading to nearly instantaneous hydrogenation, we can effectively simulate the physical growth of an ice mantle by depositing end-product molecules directly during a gradual cooling process. Under these realistic conditions, using a three component mixture, H_2O, NH_3 and CO, we find that ices develop an intrinsic molecular segregation: H_2O and NH_3 condense first, followed by a CO-rich outer shell that only forms as temperatures drop below 30 K.

This research was conducted using two complementary ultra-high vacuum facilities: the Light Irradiation Facility for Exochemistry (LIFE) at INAF-Osservatorio Astronomico di Palermo and the Interstellar Energetic-Process System (IEPS) at the National Central University in Taiwan. Both facilities are centered around an ultra-high vacuum (UHV) chambers coupled with in situ Fourier-transform infrared (FTIR) spectroscopy and Quadrupole Mass spectrometry (QMS) to monitor the evolution of ices at cryogenic temperatures. The primary differences between them lie in their irradiation sources. While both laboratories are equipped with hydrogen discharge lamps to produce vacuum-ultraviolet (VUV) photons, for simulating the interstellar radiation field, they differ in their high-energy source capabilities. LIFE is equipped with an electron-impact X-ray source for studying high-energy processing in circumstellar environments, whereas IEPS utilizes a direct electron gun. This electron source is used to simulate both

the ionization chemistry induced by cosmic rays in deep space or the electron irradiation of icy moons orbiting giant planets in the Solar System, where energetic particles from planetary magnetospheres constantly process surface material.

Because infrared line profiles serve as precise indicators of physical processes and chemical interactions to which a molecule is subjected, a suite of 18 experiments was conducted at the IEPS facility in Taiwan, utilizing two distinct deposition protocols across various deposition pressures and molecular combinations of the molecular species H2O, NH3, CH4, CO, CO2, and CH3OH . For this specific stage of the work, no external energy sources were employed, focusing exclusively on the physical accretion and condensation processes to ensure that the resulting structural data reflects pristine formation conditions. By decomposing the laboratory CO stretching mode into specific Gaussian profiles, we established a diagnostic framework capable of identifying unique molecular micro-environments. This library has been used as a tool to translate the complex line profiles observed by the James Webb Space Telescope (JWST) into a direct understanding of ice structure. When applied to high-resolution JWST data, our framework reveals a stark contrast in ice evolution: while molecular cloud sightlines show evidence of neat stratification, protoplanetary disk spectra indicate more heterogeneous, mixed, or reprocessed ices. This transition reflects the dynamic nature of disks, where turbulence and snow-line crossings blur the original layers, and demonstrates that the structural history of ice is fundamentally preserved in its infrared signature. Notably, our analysis demonstrates that although the library is extensive, only four primary Gaussian components are required to reproduce the observed CO features in astronomical spectra, with two of these components being common to all modeled sources.

While the macroscopic architecture of ice, whether layered or mixed, is a primary driver of chemical evolution, the underlying template upon which these ices condense may also play a significant role. To explore this, we extended our laboratory simulations beyond inert substrates to include the use of ground meteoritic material as a proxy for innterplanetary dust particles. This allowed us to investigate the interfacial dynamics between the mineral surface and the ice mantle, specifically looking for evidence of surface-mediated structural changes that occur during the accretion. Comparative analysis reveals that while CO ice deposited on inert ZnSe at 10 K remains predominantly amorphous, the presence of a meteoritic backbone induces a multi-component infrared profile characterized by a distinct blue-shifted shoulder. We propose that this feature arises from the high rugosity and intrinsic mineralogy of the meteorite, which provide specific adsorption sites that act as a physical template. These sites appear to facilitate a more ordered molecular
arrangement than is typically observed on flat, inert surfaces at 10 K, altering the physical architecture of ice mantles. If robustly confirmed, the nature of the condensing surface should be considered when interpreting the high-resolution spectroscopic signatures of cold astrophysical environments.

The final phase of this work extends the investigation to planetary surfaces, specifically examining the radiolytic processing of sodium orthophosphates (Na3PO4) as a proxy for the icy crust of Enceladus. This rersearch has been troggered by the 2023 Cassini discovery of soluble sodium orthophosphates in Enceladus's plumes that revealed concentrations up to 1,000 times higher than Earth's oceans, significantly strengthening the moon's
prebiotic potential. Utilizing electron and X-ray irradiation to simulate magnetospheric bombardment, we show that stable mineral salts act as active chemical sites rather than inert substrates. Our results show that radiolysis induces localized structural disorder and symmetry breaking within the phosphate lattice, facilitating the conversion of orthophosphates into hydrogen phosphates, a critical step in the formation of prebiotic energetic backbones. Furthermore, when processed in the presence of H2O and CO ices, the phosphate surface stabilizes complex photoproducts, including formaldehyde and methanol, and promotes the chemical binding of water at temperatures up to 300 K. These findings suggest that the interaction between ionizing radiation and mineral surfaces is a fundamental driver for the synthesis and preservation of prebiotic precursors on icy moons, bridging the gap between simple astrophysical ices and the building blocks of life. Future work will expand upon these findings, investigating the formation of reactive defect centers, the condensation of pyrophosphates and the phosphorus incorporation into organic compounds.

Rashida Aslam
PhD studdent

The PhD Board Dean.

Prof. Marco Cannas

Allegato 6

PHD IN PHYSICAL AND CHEMICAL SCIENCES, XXXVIII COURSE

PhD Candidate: Marco Vetrano

Transcript of Records

Tutor: Massimo Palma

Cotutor: Salvatore Lorenzo

Courses/school/exam scores:

- Quantum Information Theory
- Agent Based Models
- Open Quantum Systems and Quantum Machine Learning

Research and training periods abroad

6 months of research at the IFISC Institute for Cross-Disciplinary Physics and Complex Systems, under the co-supervision of Roberta Zambrini and Gian Luca Giorgi, from the 01-02-2025 to 15-07-2026. During this period I worked on studying the relation between the performances of Quantum Reservoir Computing and Generalized Synchronization phenomena.

Papers published:

- Vetrano, Marco, et al. "State estimation with quantum extreme learning machines beyond the scrambling time." *npj Quantum Information* 11.1 (2025): 20.
- Vetrano, Marco, et al. "Exoplanetary atmospheres retrieval via a quantum extreme learning machine." *arXiv preprint arXiv:2509.03617* (2025). (Under peer review at Quantum Machine Intelligence)
- **Vetrano et al. "Optimized Quantum Extreme Learning Machine for Supernovae Remnant Spectral Analysis" (in preparation)**

Conferences/workshop attended:

- **Talks:**
- **Information scrambling in quantum tomography performed with quantum extreme learning - New Trends in Non-Equilibrium Statistical Mechanics 2023**
- *QELM response to scrambling dynamics and applications for atmospheric retrieval.* - **Quantum Reservoir Computing Working Party**
- **Exoplanetary Atmospheres Retrieval via a quantum extreme learning machine – SIF25**
- **Winner of the First prize at QuHack4AI – Quantum Hackaton for Industrial Applications in September 2024 (no talks)**
- **Attended at EQAI Summer School in Udine in June 2023 (no talks)**

- Posters:
  - Information scrambling in quantum tomography performed with quantum extreme learning – QTML2023
  - State estimation with quantum extreme learning machines beyond the scrambling time – IQIS24
  - Exoplanetary Atmospheres Retrieval via a quantum extreme learning machine – IQIS25

Thesis title:
Noise-Resilient Quantum Extreme Learning Machines for Astrophysical Spectral Analysis
Abstract:

In this thesis we investigate the information processing capabilities of Quantum Extreme Learning Machines and discuss their real world applications in the field of astrophysics, particularly for atmospheric retrieval of exoplanets and supernovae spectral analysis, designing noise resilient models for Noise Intermediate Scale Quantum (NISQ) implementations.

Extreme Learning Machines (ELMs) offer rapid training and structural efficiency by utilizing a randomized hidden layer—the reservoir—to map input data into a high-dimensional feature space, effectively linearizing complex learning problems. While traditionally implemented via randomized classical neural networks, the mathematical properties of these reservoirs naturally extend to complex physical systems. This universality has driven the development of Quantum Extreme Learning Machines (QELMs), which utilize quantum systems as the computational reservoir. In the field of physical extreme learning machines, information is processed through the internal dynamics of the system and recollected by measuring the system. In the context of QELMs, this consists in selecting a set of observables or a POVM to be measured on the reservoir, whose outcomes is then used to train the post-processing layer.

In this work, we will first review the foundations of Neural Networs, ELMs and Reservoir Computers, highlighting specifically on similarities and fundamental differences between these models and develop the theory behind the quantum counterparts. Then, we demonstrate that QELMs can efficiently process and estimate quantum states well beyond the reservoir's scrambling time, beyond which the information should be irretrievable through local measurements. Furthermore, we show that within this regime, specific classes of Hamiltonians achieve reconstruction accuracies matching those of global random unitary dynamics. Following these theoretical aspects, we design noise-resilient QELM architectures tailored for the spectral analysis of complex astrophysical phenomena. We apply these models to exoplanetary atmospheric retrieval and supernova remnant datasets, particularly deploying the algorithm for the exoplanetary context on real quantum hardware (IBM Fez). By evaluating various pre-processing and encoding strategies—including Dense Angle Encoding, IQP embedding, and Data Re-uploading—we demonstrate that these noise-resilient QELMs are highly adaptable to different classes of astrophysical objects and capable of extracting critical spectral parameters also on NISQ devices, paving the way for real world applications of Quantum Computing in the astrophysical field.

The PhD Board Dean

Prof. Marco Cannas

Marco Cannas