Giovanni Caldarelli

POSTDOCTORAL EXPERIENCE

Nov 2024- Present **Research fellowship (assegno di ricerca, 1 year contract)**

Project: European Research Council project "ERC-Synergy More-TEM"

Principal investigator: prof. Francesco Mauri

EDUCATION AND TRAINING

Nov 2021-Nov 2024 **PhD in Physics, Sapienza University of Rome (Italy)**

Thesis title: Thermal and dynamical response of solids within and beyond perturbation theory

Advisors: prof. Francesco Mauri, Prof. Lara Benfatto

Thesis defense: 24/01/2025, Full marks and honors

Oct 2018-Oct 2020 **Master degree in Physics, Sapienza University of Rome (Italy)**

Advisors: Prof. Lara Benfatto

Thesis title: Thermal transport in complex crystals, Final Grade: 110/110 with honors

Oct 2015- Oct 2018 **Bachelor degree in Physics, Sapienza University of Rome (Italy)**

Advisors: Prof. Tullio Scopigno

Thesis title: Hartree-Fock approximation for Hydrogen molecule, Final Grade: 110/110 with honors

Sep 2010- Jul 2015 **High School, "Liceo Ginnasio Statale Orazio", Rome (Italy)**

Final Grade: 90/100

LANGUAGE SKILLS

Italian (Native), English (Advanced), Spanish (Basic)

ACADEMIC PROFILE

Prizes and awards

Scolarships PhD scholarship in "Physics PhD School Vito Volterra" at "La Sapienza", University of Rome, Italy (Accepted position).

PhD scolarship in "Theory and numerical simulation of Condensed Matter" at SISSA, Trieste, Italy (Offered position).

Excellence program of Master Degree in Physics at "La Sapienza" University of Rome, Italy (10% student accepted). The scolarship value was equal to the university fee ($\simeq$1000€).

Research grants "Avvio alla ricerca" awarded by "La Sapienza" University of Rome for early career researchers. Awarded: 2000€ in research funds (2023)

High-performance computing calls ISCRA C call (CINECA) - accepted project "Thermal Transport in Anharmonic Systems (TheTrAhs)", 100 000 CPU hours (2022)

Organized events

Workshop "Ions in motion: innovative models for heat and charge transport in insulators", main proposer of minicolloquium within FisMat 2025 conference, (Venice, Italy, to be held in Jul 2025)

Talks

Invited 22nd International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods (ICTP, Trieste, Italy, Jan 2025)

CECAM - Green's function methods: the next generation 6 (Toulouse,France Oct 2024)

European Theoretical Spectroscopy Facility (ETSF) (Webinar, Oct 2022)

Contributed CMT@BRIXEN The meeting of the condensed matter theory Italian community (Brixen, Italy, August 2024)

Attended events

Jul 2023 Stochastic Self-Consistent Harmonic Approximation (SSCHA) 2023 school in San Sebastian - attendee

Jun 2023 Condensed Matter Theory (CMT) at Brixen, meeting of the condensed matter theory Italian community - attendee

Jan 2023	21st International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods at ICTP Trieste - **Poster presentation**
Dec 2022	CECAM Mixed-Gen Season 3, Theory and numerical simulation of transport processes in condensed matter (online) - attendee
Sep 2022	MORE-TEM project workshop (Universitat Wien) - attendee
Aug 2022	Psi-k 2022 conference at SwissTech Convention Center, EPFL, Lausanne (Switzerland) - **Poster presentation**
Dec 2021	CECAM workshop: Capturing Anharmonic Vibrational Motion in First-Principles Simulations - attendee
May 2021	MaX School on Advanced Materials and Molecular Modelling with Quantum ESPRESSO (online) - attendee

Teaching and supervising

Supervising	Master degree in Physics, Sapienza University of Rome Thesis title: Relativistic corrections to LO-TO splitting, Advisor: Lara Benfatto, Candidate: Francesco Valerio Servilio (graduated with full marks and honors)
Teaching	Assistant lecturer, Classical mechanics and thermodynamics (Fisica I), bachelor degree in Mechanical Engineering, Sapienza University of Rome. Main Lecturer: Marco Rossi. 40 hours course. (Mar 2022 - Jul 2022) Assistant lecturer, General physics (Fisica Generale), bachelor degree in Environmental Sciences, Sapienza University of Rome. Main Lecturer: Alessandro Nucara. 20 hours course. (Nov 2021 - Feb 2022)

Academic Details

Review activity	I have been selected as peer reviewer of the American Physical Society (Physical Review B, 8 papers), Elsevier Editorial (Acta materialia, 1 paper), Nature Publishing Group (Nature communications, 1 paper)
Metrics	Google Scholar- Citations: 69, h-index: 3 Research Gate- Citations: 76, h-index: 2, Research interest score: 67.1
ORCID	0000-0001-8524-1273

LIST OF PUBLICATIONS

2024	**Variational formulation of dynamical electronic response functions in Bethe-Salpeter,(screened) Hartree-Fock, Hybrid-DFT approaches** G Caldarelli, A Guandalini, F Macheda, F Mauri https://arxiv.org/abs/2410.22889
	High-and low-energy many-body effects of graphene in a unified approach A Guandalini, G Caldarelli, F Macheda, F Mauri https://arxiv.org/abs/2409.17645
	Lattice thermal conductivity in the anharmonic overdamped regime Đ Dangić, G Caldarelli, R Bianco, I Savić, I Errea https://arxiv.org/abs/2410.13485
2023	**Wigner Gaussian dynamics: simulating the anharmonic and quantum ionic motion** A Siciliano, L Monacelli, G Caldarelli, F Mauri Physical Review B 107 (17), 174307 (2023), DOI:https://doi.org/10.1103/PhysRevB.107.174307
2022	**Many-body Green's function approach to lattice thermal transport** G Caldarelli, M Simoncelli, N Marzari, F Mauri, L Benfatto Physical Review B 106, 024312 (2022), DOI: https://doi.org/10.1103/PhysRevB.106.024312

ADDITIONAL INFORMATION

Software skill	I have extended knowledge of Python coding language for scientific programming. I have experience of software for materials modeling and simulation of solid state physics as QUANTUM ESPRESSO, Phonopy, Phono3py.
Work experience	**Student orientation and information desk**, Sapienza University of Rome, two 150h work contracts with the Physics Department
Volunteering and Social activities	Activities and formation activities as scout leader in AGESCI organization (until 2016)
	High school representative for the district student council (consulta provinciale) (2015)
Hobbies and sports	Climbing and hiking, guitar player enthusiast