

## SCIENTIFIC PROFESSIONAL CURRICULUM

FRANCESCO MACHEDA

### PART I - GENERAL INFORMATION

<b>Name and surname</b>	Francesco Macheda
<b>Date of birth</b>	30/08/1992
<b>Place of birth</b>	Pisa
<b>Citizenship</b>	Italian
<b>Currently held academic position</b>	Tenure Track (RTT) Researcher, University of Modena and Reggio Emilia
<b>Language skills</b>	Italian, English

### PART II - QUALIFICATIONS/EMPLOYMENT CONTRACTS

<b>Title</b>	<b>Duration/Achievement</b>	<b>Institution</b>	<b>Assessment</b>	<b>Note</b>
Scientific high school diploma	2005-2010	A. Pacinotti Scientific High School, La Spezia	100/100 like praise	
Bachelor's Degree in Physics	28/02/2014	University of Pisa, Italy	110/110 how praises	
Master's Degree in Physics	24/10/2016	University of Pisa, Italy	110/100 like praise	<b>Thesis:</b> Strain engineering of germanium surface states: an ab-initio study. <b>PI</b> :Prof. Giuseppe Grosso
PhD in Physics	01/07/2021	King's College London, UK		<b>Thesis:</b> Ab initio prediction of thermomagnetic and thermoelectric transport phenomena in 3d and 2d materials.

				<b>Speaker:</b> Dr. Nicola Bonini
Postdoc (Collaborator)	01/02/2021-31/05/2023	Italian Institute of Technology		<b>Scientific Director:</b> Prof. Francesco Mauri
Postdoc (Assistant)	01/06/2023-15/01/2024	University of Rome La Sapienza		<b>Scientific Director:</b> Prof. Francesco Mauri
Type A fixed-term researcher (RTDA)	15/01/2024-01/03/2025	University of Rome La Sapienza		<b>Scientific Director:</b> Prof. Francesco Mauri
Tenure Track Researcher (RTT)	01/03/2025-In progress	University of Modena and Reggio Emilia		

### PART III - ELEMENTS SUBJECT TO EVALUATION

#### A) PUBLICATIONS

**IF WOS** = Impact Factor **INeb THEf Science**

For more recent articles from 2022, the **IF** of the newspaper relating to 2022.

N.	Typology	Authors	Title	Magazine	Year	IF WOS	Notes
23	Journal Article	Cangpeng Lin, Samuel Poncé, <b>Francesco Macheda</b> , Francesco Mauri, Nicola Marzari	Elastic Constants and Bending Rigidities from Long-Wavelength Perturbation Expansions	arXiv	2024		
22	Journal Article	JohnCaldarelli, Alberto Guandalini, <b>Francesco Macheda</b> , Francesco Mauri	Variational formulation of dynamical electronic response functions in Bethe-Salpeter,	Physical Review B 111, 075137	2025		

			(screened) Hartree-Fock, Hybrid-DFT approaches				
21	Journal Article	Alberto Guandalini, Giovanni Caldarelli, <b>Fr ancesco Macheda</b> , Francesco Mauri	High- and low-energy many-body effects of graphene in a unified approach	Physical Review B 111, 075118	2025		
20	Journal Article	Paolo Fachin, <b>Francesco Macheda</b> , Paolo Barone, Francesco Mauri	Nearly quantized Born effective charges as probes for the topological phase transition in the Haldane and Kane-Mele models	Physical Review B, 110, L201405	2024	3.7 (2022)	Editor's suggestion

19	Journal Article	<b>Francesco Macheda</b> , Paolo Barone, Francesco Mauri	First principles calculations of dynamical Born effective charges, quadrupoles and higher order terms from the charge response in large semiconducting and metallic systems	Physical Review B, 110, 094306	2024	3.7 (2022)	
18	Journal Article	<b>Francesco Macheda</b> , Francesco Mauri, Thibault Sohier	Ab-initio Van der Waals electrodynamic s: polaritons and electron scattering from plasmons and phonons in BN-capped graphene	Physical Review B, 110, 115407	2024	3.7 (2022)	
17	Journal Article	Lorenzo Graziotto, <b>Francesco Macheda</b> , Thibault Sohier, Matteo Calandra, Francesco Mauri	Theory of infrared double-resonance Raman spectrum in graphene: The role of the zone-boundary electron-phonon enhancement	Physical Review B, 109, 075420	2024	3.7 (2022)	First theoretical physicist in the list of authors.
16	Journal Article	Lorenzo Graziotto, <b>Francesco Macheda</b> , Tommaso Venanzi, Guglielmo Marchese,	Infrared Resonance Raman of Bilayer Graphene: Signatures of Massive Fermions and	Nano Letters 2024, 24, 6, 1867–1873	2024	10.8 (2022)	First theoretical physicist in the list of authors.

		Simone Sotgiu, Taoufiq Ouaj, Elena Stellino, Claudia Fasolato, Paolo Postorino, Marvin Metzelaars, Paul Kögerler, Bernd Beschoten, Matteo Calandra, Michele Ortolani, Christoph Stampfer, Francesco Mauri, Leonetta Baldassarre	Band Structure on the 2D Peak				
15	Journal Article	John Marini, William Marchese, Gianni Profeta, Jelena Sjakste, <b>Francesco Macheda</b> , Nathalie Vast, Francesco Mauri, Matteo Calandra	EPIq : an open-source software for the calculation of electron-phonon interaction related properties	Computer Physics Communications Volume 295, 108950	2024	6.2 (2022)	
14	Journal Article	Guglielmo Marchese, <b>Francesco Macheda</b> , Luca Binci, Matteo Calandra, Paolo Barone, Francesco	Born effective charges and vibrational spectra in superconducting and bad conducting metals	Nature Physics, 1745-2481	2023	19.5 (2022)	

		Mauri.					
13	Journal Article	Thomas Venanzi, Lorenzo Graziotto, <b>Francesco Macheda</b> , Simone Sotgiu, Taoufiq Ouaj, Elena Stellino, Claudia Fasolato, Paolo Postorino, Vaidotas Mišeikis, Marvin Metzelaars, Paul Kögerler, Bernd Beschoten, Camilla Coletti, Stefano Roddaro, Matteo Calandra, Michele Ortolani, Christoph Stampfer, Francesco Mauri, Leonetta Baldassarre	Probing enhanced electron-phonon coupling in graphene by infrared resonance Raman spectroscopy	Physical Review Letters, 130, 256901	2023	8.6 (2022)	Editor's suggestion  First theoretical physicist in the list of authors.
12	Journal Article	<b>Francesco Macheda</b> , Thibault Sohier, Paolo Barone and Francesco Mauri	Electron-phonon interaction and phonon frequencies in two-dimensional doped semiconductors	Physical Review B 107, 094308	2023	3.7 (2022)	
11	Journal Article	Hyungjun Lee, Samuel Poncé, Kyle	Electron-phonon physics from first principles using the EPW	npj Computational Materials 9,	2023	9.7 (2022)	

		Bushick, Samad Hajinazar, Jon Lafuente-Ba rtolome, Joshua Leveillee, Chao Lian, Jae-Mo Lih, <b>Francesco Macheda</b> , Hitoshi Mori, Hari Paudyal, Weng Hong Sio, Sabyasachi Tiwari, Marios Zacharias, Xiao Zhang, Nicola Bonini, Emmaouil Kioupakis, Elena R. Margin & Feliciano Justin	code	156			
10	Journal Article	<b>Francesco Macheda</b> , Paolo Barone and Francesco Mauri	Electron-Phono n Interaction and Longitudinal-Tr ansverse Phonon Splitting in Doped Semiconductor s	Physical Review Letters 129, 185902	2022	8.6	Editor's suggestion
9	Journal Article	Simone Sotgiu, Thomas Venanzi, <b>Fra ncesco Macheda</b> , Elena Stellino, Michele Ortolani, Paolo Postorino,	Raman scattering with infrared excitation resonant with the MoSe2 indirect band gap	Physical Review B 106, 085204	2022	3.7	First and only theoretical physicist in the list of authors.

		and Leonetta Baldassarre					
8	Conference paper	Simone Sotgiu, Thomas Venanzi, <b>Francesco Macheda</b> , Elena Stellino, Paolo Postorino, Michele Ortolani, and Leonetta Baldassarre	Raman scattering with near infrared excitation selectively resonant with the indirect bandgap of bulk MoSe2	International Conference on Infrared, Millimeter, and Terahertz Waves, IRMMW-T Hz, Volume 2022	2022		First and only theoretical physicist in the list of authors.  IF not available.
7	Journal Article	Evgeny Plekhanov, Zelong Zhao, <b>Francesco Macheda</b> , Yao Wei, Nicola Bonini, Cedric Weber	Computational Materials Discovery for Lanthanide Hydrides at high pressure: predicting High Temperature superconductivity	Physical Review Research 4, 013248	2022	4.2	
6	Journal Article	Yao Wei, <b>Francesco Macheda</b> , Zelong Zhao, Terence Tse, Evgeny Plekhanov, Nicola Bonini and Cedric Weber	High-Temperature Superconductivity in the Lanthanide Hydrides at Extreme Pressures	Applied Sciences 2022, 12(2), 874	2022	2.7	
5	Journal Article	Samuel Ponce, <b>Francesco Macheda</b> , Elena Roxana Margine,	First-principles predictions of Hall and drift mobilities in semiconductors	Physical Review Research 3, 043022	2021	4.2 (2022)	The only IF available for Physical Review Research

		Nicola Marzari, Nicola Bonini and Feliciano Justin					is for 2022.
4	Journal Article	G. Gagliardi and <b>F. Macheda</b>	Spinodal-assisted nucleation in the two-dimensional $q$ – state Potts model with short-to-long-range interactions	Physical Review E 104, 014115	2021	2.707	
3	Journal Article	<b>F. Macheda</b> , S. Poncè, F. Giustino and N. Bonini	Theory and computation of Hall scattering factor in graphene	Nano Letters 2020, 20, 12, 8861–8865	2020	11.189	
2	Journal Article	Cone of Paola, <b>Francesco Macheda</b> , Savio Laricchia, Cedric Weber, and Nicola Bonini	First-principles study of electronic transport and structural properties of Cu <sub>12</sub> Sb <sub>4</sub> S <sub>13</sub> in its high-temperature phase	Physical Review Research 2, 033055	2020	4.2 (2022)	The only IF available for Physical Review Research is for 2022.
1	Journal Article	<b>F. Macheda</b> and N. Bonini	Magneto-transport phenomena in p-doped diamond from first principles	Physical Review B 98, 201201(R)	2018	3.736	

## B) TEACHING

Period	Institution and status	Description
First half of 2017	King's College London, UK	Teaching assistant for the course “Classical mechanics”. Instructor: Dr. Furqaan Yusaf (15 hours of frontal teaching).

Second half of 2017	King's College London, UK	Teaching assistant for the course "Computational laboratory". Instructor: Prof. Francesca Baletto (15 hours of frontal teaching)
Second half of 2018	King's College London, UK	Teaching assistant for the course "Computational laboratory". Instructor: Prof. Francesca Baletto (15 hours of frontal teaching).
March 4, 2024 - June 15, 2024	University of Rome La Sapienza, Italy	Holder of the course "Physics" for the degree course in Biological Sciences. 27 hours of frontal teaching and 350 hours of teaching and student support
September 30, 2024 - December 18, 2024	University of Rome La Sapienza, Italy	Teacher of the course "Computational Physics 1" for the degree course in Physics. 36 hours of frontal teaching and 350 hours of teaching and student support

### C) RESEARCH, ORGANIZATIONAL, MANAGEMENT AND SERVICE ACTIVITIES

#### Documented training or research activity at qualified Italian or foreign institutions:

Role	Period	Institution	Description
PhD	01/01/2017-01/01/2021	King's College London	<b>Goal:</b> Study of charge and heat transport properties by solving the Boltzmann equations of electrons and phonons, with applications to materials of technological importance. <b>Scientific Director:</b> Dr. Nicola Bonini
Postdoc (Collaborator)	01/02/2021-31/05/2023	Italian Institute of Technology, Italy	<b>Goal:</b> Implement the tasks of Work-Package 1 Enabling Science which aims at exploring new fundamental research fields in graphene and 2D materials by developing the project

			related to characterization and modeling to control the properties of materials and to search for new effects in graphene, BN and TMSs within the CORE3 project EPUE0249. <b>Scientific Director:</b> Prof. Francesco Mauri
Postdoc (Assistant)	01/06/2023-15/01/2024	University of Rome La Sapienza, Italy	<b>Goal:</b> Theory and first-principles calculation of phonons and their fluctuations of charge, in metals, doped semiconductors and insulators – applications to electron-phonon interaction and to the simulation of inelastic electron scattering spectroscopy <b>Scientific Director:</b> Prof. Francesco Mauri
Type A fixed-term researcher (RTDA)	01/15/2024- In progress	University of Rome La Sapienza, Italy	<b>Goal:</b> First-principles theory and computation of phonons and their charge fluctuations, adiabatic and non-adiabatic, in metals, doped semiconductors and insulators—applications to electron-phonon interaction and simulation of inelastic electron scattering spectroscopy (EELS) <b>Scientific Director:</b> Prof. Francesco Mauri

**Organization, direction and coordination of national and international research groups, or participation in the same:**

**PI = Principal Investigator/Responsabile**

**Co-PI = Co-Responsible**

Period	Research program	Role held
2023-2025	Member of the project “MORE-TEM ERC-SYN grant agreement no. 95121”	Postdoc e RTDA

2021-2023	Membro del progetto “European Union’s Horizon 2020 research and innovation program under Grant Agreements No. 881603-Graphene Core3”	Postdoc
2024-2025	EuroHPC Regular Access Call — Prediction of high-Tc superconducting hydrides at ambient pressure, lead by Prof. Ion Errea, University of the Basque Country, Spain, awarded 14,462,208 standardized CPU hours	Co-PI
2023-2024	EuroHPC Call 2022— Exploring competing broken symmetry states in quantum anharmonic materials lead by Prof. Matteo Calandra, University of Trento, Italy, awarded 30,000,000 standardized CPU hours	Co-PI
2021-2022	PRACE call—OptoSpin led by Prof. Matthieu Verstraete, University of Liège, Belgium awarded of 40,000,000 standardized CPU hours for each of the three years duration	Collaborator
2020-2021	DECI-16 PRACE— MATROMUGR (MAGneto-TRANsport properties Of MULTilayer GRAPHitic structures) awarded of 14,000,000 standardized CPU hours	PI
2019-2020	EPSRC Tier 2 RAP—Thermoelectric properties of SnSe from first-principles lead by Dr. Nicola Bonini, King's College London, UK awarded 2,000,000 standardized CPU hours	Collaborator
2017	EPSRC ARCHER RAP—Transport coefficients in Diamond and Silicon-Carbides lead by Dr. Nicola Bonini, King's College London, UK awarded 1,800,000 standardized CPU hours	Collaborator
2017-In progress	ISCRA-C Projects IsC53_Ge-Surf IsCc4_PAWBEC IsCb5_irlah IsCa9_RSHAS IsCa9_BEGRRA IsCa6_dop-EELS IsCa4_TheTrAhS IsC95_HsymX IsB22_HPMETH	Collaborator

2018-2023	Computational infrastructure developer for the “EPW” code ( <a href="https://epw-code.org/">https://epw-code.org/</a> ), focused on the calculation of electron-phonon interaction from first principles	Developer
2023-In progress	Computational infrastructure developer for the “Epiq” code ( <a href="https://the-epiq-team.gitlab.io/epiq-site/">https://the-epiq-team.gitlab.io/epiq-site/</a> ), focused on the calculation of electron-phonon interaction from first principles	Developer
2021-In progress	Active collaboration with various experimental groups present at the University of Rome La Sapienza, and other international groups as demonstrated by the 5 publications (numbered 1,2,5,9,10) with experimental physicists in the list of authors.	
2024-onward	FAR of studies 2025, DISMI, Universities of Modena and Reggio Emilia – PI Small and medium projects 2024, Faculty of Physics, University of Rome La Sapienza – Participant	

**Speaker at national and international conferences and conventions:**

Data	Site	Conference title	Participation type
09/05/2025	Online	ETSF Webinar	<b>Invited Speaker.</b> <b>Titolo:</b> Coupling Plasmons and Polar Phonons in van der Waals Heterostructures: Theory and Transport Implications
23/09/2024	Louvain-la-Neuve, Belgium	ETSF Electron-phonon collaboration team workshop	<b>Invited Speaker.</b> <b>Titolo:</b> First principles calculations of dynamical quadrupoles and higher order terms from the density response in large

			semiconducting and metallic systems
28/08/2024	Brixen, Italy	CMT@Brixen	<b>Invited Speaker.</b> <b>Titolo:</b> First principles calculations of dynamical quadrupoles and higher order terms from the density response in large semiconducting and metallic systems
11/04/2024	London, United Kingdom	Frontiers in Thermal and Electronic Transport in Materials: A Tribute to Nicola Bonini	<b>Invited Speaker.</b> <b>Titolo:</b> The significance of screening effects in the electron-phonon coupling of doped semiconductors
26/03/2024	Osaka, Japan	MORE-TEM Symposium 2024	<b>Contributed talk.</b> <b>Title:</b> Van der Waals heterostructures from ab-initio: plasmon, phonons and phonon-polariton dispersions
12/01/2023	Trieste, Italy	21st International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods	<b>Invited speaker.</b> <b>Titolo:</b> Effective charges, electron-phonon interaction and infrared spectroscopy in doped semiconductors, metals and hydrogen-based high-Tc superconductors
24/08/2022	Lausanne, Switzerland	International conference on thermoelectric materials	<b>Contributed talk.</b> <b>Titolo:</b> Electron phonon interaction in two and three-dimensional doped semiconductors

18/03/2022	Chicago, USA	APS March Meeting 2022	<b>Contributed talk.</b> <b>Titolo:</b> Wannier interpolation of electron-phonon coupling in doped semiconductors
13/09/2021	Online	107th National Congress of the Italian Physical Society	<b>Communication.</b> <b>Title:</b> First-principles predictions of transport properties via the Boltzmann approach
01/05/2019	London, United Kingdom	UK thermoelectric network meeting	<b>Contributed Talk.</b> <b>Title:</b> Electrons and phonons from density functional theory
13/06/2019	San Sebastian, Spain	International conference on thermoelectric materials	<b>Contributed talk.</b>

**Seminars, poster presentations, and other activities:**

<b>Data</b>	<b>Site</b>	<b>Conference title</b>	<b>Participation type</b>
2024	Trieste, Italy	22nd International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods	<b>Poster</b>
2023	Rome, Italy	Department seminar for RTDA call D.D. 145/23, University of Rome La Sapienza	<b>Seminar</b>
2023	Brixen, Italy	CMT Brixen	<b>Poster</b>
2021	Trieste, Italy	20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods	<b>Poster</b>

2021	Online	EPW Virtual Summer School	<b>Panelist and teaching assistant</b>
2019	London, United Kingdom	TYC student day	<b>Poster</b>
2018	Trieste, Italy	School on Electron-Phonon Physics from First Principles	<b>Poster</b>

Various internal seminars within the research groups/participatory projects are not reported.

**Additional titles held:**

<b>Title</b>	<b>Date of performance</b>	<b>Description</b>
Official co-supervisor of the doctoral thesis	In progress	Supervision of the scientific activity during the PhD thesis of Paolo Fachin, University of Rome La Sapienza
Official co-supervisor of master's thesis	A.A. 2020-2021	<b>Thesis:</b> Experimental and ab-initio resonant Raman of graphene with infrared excitation <b>Students:</b> Lorenzo Graziotto <b>Vote:</b> 110/110 how praises
Official co-supervisor of master's thesis	A.A. 2021-2022	<b>Thesis:</b> Identification of stacking order in multilayer graphene by resonant Raman spectroscopy <b>Students:</b> Gregory Staffieri <b>Vote:</b> 110/110 how praises
Reviewer for journals scientific	In progress	
Reviewer for ISCRA-Cineca projects	In progress	
Co-supervisor for Bachelor's and Master's theses	In progress	Triennials: Alessandro Di Simone Masters: Raffaele Narciso At the University of Rome La Sapienza
Member of the Master's Degree Committees	In progress	Sessions: 10/30/2024, 01/27/2025

		At the University of Rome La Sapienza
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## BIBLIOMETRIC INDEXES

Academic seniority	8 years (2025-2018+1)
ORCID	0000-0001-8255-7838

### Bibliometric indices according to Scopus (01/03/2024)

**NB:** Conference papers are not counted in the following calculation

Index	Total
Number of publications	16
Quotations	160
Average citations per publication	10
Hirsh index (h-index)	7
Total impact factor	107.432
Average impact factor per research item	6.715

### Bibliometric indices according to Google Scholar (01/06/2024)

Index	Total
Quotations	236
Hirsh index (h-index)	7

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Rome, there

In faith  
Francesco Macheda