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# Francesco Macheda

**Date of birth:** | **Nationality:**Italian | **Gender:** Male | **Phone number:** ( Mobile) |

**Email address:** | **Email address:** |

**Address:**

## EDUCATION AND TRAINING

2005 – 2010 La Spezia, Italy

**HIGH SCHOOL DEGREE**Liceo scientifico A. Pacinotti

**Address**

| **Final grade**100/100 cum laude

La Spezia, Italy 28/02/2014 Pisa, Italy

**BACHELOR DEGREE IN PHYSICS** Univeristà di Pisa

**Address**

| **Final grade**110/110 cum laude

Pisa, Italy 24/10/2016 Pisa, Italy

**MASTER DEGREE IN THEORETICAL PHYSICS** Università di Pisa

**Address** Pisa, Italy | **Final grade**110/110 cum laude |

**Thesis** Strain engeneering of germanium surface states: an ab-initio study. PI : Prof. Giuseppe Grosso

01/07/2021 London, United Kingdom

**PHD IN PHYSICS** King's College London

**Address** London, United Kingdom |

**Thesis** Ab initio prediction of thermomagnetic and thermoelectric transport phenomena in 3d and 2d materials

01/02/2021 – 31/05/2023

**COLLABORATOR (CO.CO.CO.) AT ISTITUTO ITALIANO DI TECNOLOGIA**

## LANGUAGE SKILLS

Mother tongue(s): **ITALIAN** Other language(s):

| | UNDERSTANDING | SPEAKING | WRITING |
|---|---|---|---|

| Listening | Reading | productionSpoken | interactionSpoken |
|---|---|---|---|
| [redacted] | | | |

*Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user*

## ADDITIONAL INFORMATION

## PUBLICATIONS

**Born effective charges and vibrational spectra in super and bad conducting metals**

Guglielmo Marchese, Francesco Macheda, Luca Binci, Matteo Calandra, Paolo Barone, Francesco Mauri.

https://doi.org/10.48550/arXiv.2303.00741

**Electron-phonon interaction and phonon frequencies in two-dimensional doped semiconductors** – 2022

Francesco Macheda, Thibault Sohier, Paolo Barone and Francesco Mauri

Phys. Rev. B 107, 094308

**Electron-phonon physics from first principles using the EPW code**

Hyungjun Lee, Samuel Ponce, Kyle Bushick, Samad Hajinazar, Jon Lafuente-Bartolome, Joshua Leveillee, Chao Lian, Francesco Macheda, Hari Paudyal, Weng Hong Sio, Marios Zacharias, Xiao Zhang, Nicola Bonini, Emmanouil Kioupakis, Elena R. Margine, and Feliciano Giustino https://doi.org/10.48550/arXiv.2302.08085

**Probing enhanced electron-phonon coupling in graphene by infrared resonance Raman spectroscopy**

– 2022

Tommaso Venanzi, Lorenzo Graziotto, Francesco Macheda, 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, Cristoph Stampfer, Francesco Mauri, Leonetta Baldassarre

Phys. Rev. Lett. XXX, Accepted 15 May 2023

**Electron-Phonon Interaction and Longitudinal-Transverse Phonon Splitting in Doped Semiconductors**

– 2022

Francesco Macheda, Paolo Barone and Francesco Mauri

Phys. Rev. Lett. 129, 185902, Editor's Suggestion

**Raman scattering with infrared excitation resonant with the MoSe2 indirect band gap** – 2022 Simone Sotgiu, Tommaso Venanzi, Francesco Macheda, Elena Stellino, Michele Ortolani, Paolo Postorino, and Leonetta Baldassarre

Phys. Rev. B 106, 085204

**Raman scattering with near infrared excitation selectively resonant with the indirect bandgap of bulk MoSe2**

– 2022

International Conference on Infrared, Millimeter, and Terahertz Waves, IRMMW-THz, Volume 2022-August2022

Simone Sotgiu, Tommaso Venanzi, Francesco Macheda, Elena Stellino, Paolo Postorino, Michele Ortolani, and Leonetta Baldassarre

**High-Temperature Superconductivity in the Lanthanide Hydrides at Extreme Pressures** – 2022 Yao Wei, Francesco Macheda, Zelong Zhao, Terence Tse, Evgeny Plekhanov , Nicola Bonini and Cedric Weber

Appl. Sci. 2022, 12(2), 874

**Computational Materials Discovery for Lanthanide Hydrides at high pressure: predicting High Temperature superconductivity**

– 2021
Evgeny Plekhanov, Zelong Zhao, Francesco Macheda, Yao Wei, Nicola Bonini, Cedric Weber

Phys. Rev. Res. 4, 013248 (2022)

**Spinodal-assisted nucleation in the two-dimensional q − state Potts model with short-to-long-range interactions**

– 2021
G. Gagliardi and F. Macheda

Phys. Rev. E 104, 014115

**First-principles predictions of Hall and drift mobilities in semiconductors** – 2021

Samuel Ponce, Francesco Macheda, Elena Roxana Margine, Nicola Marzari, Nicola Bonini and Feliciano Giustino

Phys. Rev. Res. 3, 043022 (2021)

**Ab initio prediction of thermomagnetic and thermoelectric transport phenomena in 3d and 2d materials**

– 2021
Ph.D. thesis

10.13140/RG.2.2.31900.00643

**Theory and computation of semi-classical Hall scattering factor in graphene** – 2020

F. Macheda, S. Poncè, F. Giustino and N. Bonini

Nano Lett. 2020, 20, 12, 8861–8865

**First-principles study of electronic transport and structural properties of Cu12Sb4S13 in its hightemperature phase**

– 2020
Cono Di Paola, Francesco Macheda, Savio Laricchia, et al.

Phys. Rev. Research 2, 033055

**Magneto-transport phenomena in p-doped diamond from first principles** – 2018

F. Macheda and N. Bonini

Phys. Rev. B 98, 201201(R)

**Strain engineering of germanium surface states: an ab-initio study.** – 2016

M.Sc. thesis

## CODE DEVELOPMENT COLLABORATIONS

CURRENT
**Active developer of the EPW software** https://epw-code.org/

CURRENT
**Active developer of the Epiq software** https://the-epiq-team.gitlab.io/epiq-site/

## AWARDED COMPUTATIONAL CALLS

2023 – CURRENT
**EuroHPC Call 2022**

Co-PI of the project Exploring competing broken symmetry states in quantum anharmonic materials lead by Prof. Matteo Calandra, Universita' di Trento, Italy, awarded of 30,000,000 standardized CPU hours.

2020 – 2022
**PRACE call 21**

Collaborator for the project OptoSpin lead by Prof. Matthieu Verstraete, University of Liège, Belgium awarded of 40,000,000 standardized CPU hours for each of the three years duration

2020 – 2021
**DECI-16 PRACE**

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PI for the project MATROMUGR (MAgneto-TRansport properties Of MUltilayer GRaphitic structures) awarded of 14,000,000 standardized CPU hours

2019 – 2020
**EPSRC Tier 2 RAP**

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Collabotor of the project Thermoelectric properties of SnSe from first-principles lead by Dr. Nicola Bonini,King's College London,UK awarded 2,000,000 standardized CPU hours

2017
**EPSRC ARCHER RAP**

Collaborator of the project Transport coefficients in Diamond and Silison-Carbides lead by Dr. Nicola Bonini,King's College London,UK awarded 1,800,000 standardized CPU hours

2017
**ISCRA C call (CINECA)**

Collaborator of Prof. G. Grosso,Università di Pisa,Italy

## TEACHING

**Teaching assistant for the course "Computational laboratory"**

Second Semester of 2017, course held by Prof. Francesca Baletto, King's College London
Second Semester of 2018, course held by Prof. Francesca Baletto, King's College London

**Teaching assistant for the course "Classical mechanics" at King's College London**

First semester of 2017, course held by Dr. Furqaan Yusaf, King's College London

## CONFERENCES, TALKS AND EVENTS

12/01/2023
**21st International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods**

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Invited Talk

2022
**Psi-k Conference 2022**

Contributed talk

2022
**APS March Meeting 2022**

Contributed talk

2021
**107° Congresso Nazionale Società Italiana di Fisica**

Communication

2019
**UK thermoelectric network meeting**

Talk

2019

**International conference on thermoelectric materials**

Talk

30/05/2022

**IIT internal seminars**

Talk

2021

**20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods**

Poster presentation

2019

**TYC student day**

Poster presentation

2018

**School on Electron-Phonon Physics from First Principles**

Poster presentation

2021

**EPW SCHOOL 2021**

Panelist and Teaching Assistant https://epw2021.oden.utexas.edu/

## PROGRAMMING

CURRENT

**Programs and languages**

I have a full knowledge of the QUANTUM ESPRESSO suite as I am an active developer of some of its parts. I am an expert of FORTAN90 with a particular focus on massive parallelization. I have good knowledge of the other most common coding languages (Python, C++) and with programs such as Wolphram Mathematica and Matlab. I also have a good knowledge of other common programs used in first-principles calculations (ABINIT, VASP, CRYSTAL).

## REFERENCE CONTACTS

CURRENT

**Prof. Francesco Mauri**

Professor of Theoretical Solid State Physics, University of Rome Sapienza -- Relation : Collaborator
francesco.mauri@uniroma1.it

**Prof. Feliciano Giustino**

Jr. Chair at University of Texas -- Relation : Collaborator
fgiustino@oden.utexas.edu 512-232-5755

## ACADEMIC DETAILS

**Academic seniority**

6 years [2023-2018+1]

**ORCID**

0000-0001-8255-7838

**Metrics**

10 published papers on peer-reviewed journals, 3 preprints (arXiv) of which one accepted on Physical Reviev Letter, and 1 conference paper. All the 10 published papers on peer-reviewed journals are meant to be considered as selected for evaluation.

Google scholar (16/05/2023):
Citations 133 H-index 5

Scopus (16/05/2023):
Citations 69
Average citations 6.9
H-index 4
Normalized H-index (divided by academic sentiority) 0.666

Web of Science (16/05/2023):
Total impact factor 37.417 (Physical Review Research, where 3 publications were published, has no impact factor yet)
Average impact factor 5.3452 (Publications without IF are excluded)

## STUDENT SUPERVISION

**Co-advisor for M.Sc. Thesis "Experimental and ab-initio resonant Raman spectra of graphene with infrared excitation"**

2020-2021 Student: Lorenzo Graziotto (Advisor: Prof. F. Mauri), Sapienza University of Rome

**Co-advisor for M.S. Thesis "Identification of stacking order in multilayer graphene by resonant Raman spectroscopy"**

2021-2022 Student: Gregorio Staffieri (Advisor: Prof. F. Mauri), Sapienza University of Rome

## RESEARCH ACTIVITIES

### Overview

My research reference field is theoretical condensed matter and solid state physics, even though my research interest are wider and include, e.g., statistical mechanics. My approach to the research activity is to individuate an open problem with broad implications in my field of interest, and then to use the tools that I have learnt during my research years, or create new ones, in order to solve it. My toolbox include a detailed knowledge of the theory of first principle techiniques, and a vast, though not specialized, knowledge of many-body techniques coming from my M.Sc. in Theoretical Physics and successive studies. Moreover, during my PhD I developed a deep knowledge of QUANTUM ESPRESSO, which is one of the most used computational infrastructure within the solid state community. I'm currently an active developer of several suites contained or connected to it (e.g. EPW or EPIq). The whole of these acquired skills let me face a research problem both from an analytical and computational point of view, the first intended to unveil the physics behind the processes of interests and the second used to quantitatively address their evalution.

### Research focus

My reasearch focus has been centered mainly on the study of the electron-phonon coupling interaction (EPI) and its implication on electric transport and magnetotransport properties, thermoelectric coefficients, Raman and infrared spectroscopy, electron energy loss spectroscopy (EELS) and superconductivity.

In particular, I have been studying the nature of the long-range components of the EPI, which arise from the long-range nature of the Coulombian potential and are of polar nature, with a particular focus on their dependence on the number of free-carriers in a crystalline system. These developments follow from the study of the phonon-induced charge density (both in adiabatic and non-adiabatic conditions), from which I could generalize the definition of Born effective charges to doped semiconductor and metals, with broad implication not only on transport coefficients but also on infrared spectroscopy and EELS.

### Core interest

My core interest lies in the evaluation of the electronic transport coeffients. My driving motivation lies in the fact that, despite the oldness of the problem, the predictability of transport properties in two and three dimensional materials in realistic condition still suffer of strong issues, coming from the difficulty of the description of the interaction between

electrons and other quasi-particles. As a matter of fact, the presence of dielectric environment, of a finite number of carriers inside the material and of non-adiabatic dynamical effect is often discarded in the ordinary evaluation of transport properties, leading to strong over- or under-estimations of the couplings. The aim of my reasearch is to fill this void and progress towards a realistic description of transport coefficient matching experimental conditions. In this perspective, Raman and infrared spectroscopy and EELS, performed in the normal or superconducting phase, are extraordinary tools in order to reveal the quasi-particles present in a system and their interaction with electrons. As such, I am actively collaborating with many researchers with both theoretical and experimental background in order to use the above listed informative tools and better describe known properties, or determine new ones, that may help understanding the microscopic nature of the interaction between electrons and the other components of crystalline systems.