

PERSONAL INFORMATION **Antonio Siciliano**APPLICATION FOR **Postdoctoral Research Associate**

EDUCATION AND TRAINING

Oct 2020-Present **PhD, Sapienza University of Rome (Italy)**

Research focus: Exploring anharmonic effects on crystals' equilibrium and out-of-equilibrium properties utilizing the Self-Consistent Harmonic Approximation (SCHA) and the Time-Dependent Self-Consistent Harmonic Approximation (TD-SCHA).

Advisors: Prof. Francesco Mauri, Dr. Lorenzo Monacelli

Oct 2018-Oct 2020 **Master degree in Physics, Sapienza University of Rome (Italy), 110/110 with honors**

Thesis title: Quantum rotational free energies of anharmonic crystals

Thesis advisor: Prof. Francesco Mauri, Dr. Lorenzo Monacelli

Oct 2015- Sept 2018 **Bachelor degree in Physics, Sapienza University of Rome (Italy), 110/110 with honors**

Thesis title: Quantum cryptography and communication.

Thesis advisor: Prof. Fabio Sciarrino

Sep 2010- Jul 2015 **High School, "Liceo Ginnasio Statale Torquato Tasso", Rome (Italy), 98/100**

LANGUAGE SKILLS

Mother tongue Italian

Other languages

| | UNDERSTANDING | | SPEAKING | | WRITING |
|---------|---------------|---------|--------------------|-------------------|---------|
| | Listening | Reading | Spoken interaction | Spoken production | |
| English | C1 | C1 | B2 | B2 | B2 |

Levels: A1 and A2: Basic user – B1 and B2: Independent user – C1 and C2: Proficient user
[Common European Framework of Reference for Languages](#)

PRIZES AND AWARDS

2023

Research grant "Avvio alla ricerca" awarded by "La Sapienza" University of Rome for early career researchers. Project "Investigation of optical and electromechanical properties of conjugated polymers with quantum and anharmonic effects", awarded 4000€ in research funds

2022

Awarded as excellent graduate student at the 2022 'Giornata del Laureato' by the association 'Fondazione Roma Sapienza'.

2020

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

PhD scholarship 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)

HPC calls
2022-2023 IS CRA C call (CINECA) - accepted project "Infrared and Raman spectra of high-pressure hydrogen" and "Calculation of Raman Spectra in highly anharmonic systems", 100000 CPU hours for each project

LIST OF PUBLICATIONS

Wigner Gaussian dynamics: simulating the anharmonic and quantum ionic motion

Antonio Siciliano, Lorenzo Monacelli, Giovanni Caldarelli, Francesco Mauri
Physical Review B 107 (17), 174307 (2023)

ACADEMIC DETAILS

TEACHING

June 2023 - November 2023

Bachelor thesis co-supervising

Bachelor degree in Physics, Sapienza University of Rome

Thesis title: Second harmonic generation within the time-dependent self-consistent harmonic approximation,

Advisor: Prof. Francesco Mauri

Candidate: Francesco Fadda (graduated with full marks and honors)

CONFERENCES, TALKS AND EVENTS

Talks

June 2023 Lecturer at the 2023 SSCHA summer school 'Raman and Infrared spectra of strongly anharmonic materials' using the Time-Dependent Self-Consistent Harmonic Approximation (TD-SCHA)

Attended events

Jun 2023 Condensed Matter Theory (CMT) at Brixen 2023 - Poster presentation

Jan 2023 21st International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods at ICTP Trieste - Poster presentation

Sept 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

ADDITIONAL INFORMATION

Software skill

I have extended knowledge of Python, Julia and C coding language for scientific programming. I have experience of software for materials modeling and simulation of solid state physics as QUANTUM ESPRESSO, and SSCHA and TD-SCHA code.