

**PERSONAL INFORMATION** Stefano Paolo Villani

**APPLICATION FOR** Concorso per Assegno di Ricerca di categoria B Tipologia I – Bando n. 305/2023 - Rep. VII/1 - Prot. 3808 del 13-11-2023

**EDUCATION AND TRAINING**

Oct 2020 - Present **PhD Candidate, Sapienza University of Rome (Italy)**  
 Advisor: Prof. Francesco Mauri  
 The focus of my research is on the development of theoretical and computational methods to predict materials properties. In particular, the main topics of my work are:  
 – the study of the electromechanical properties of 1D systems, e.g. conjugated polymers;  
 – the effects of quantum anharmonicity on the structural and electronic properties of 1D systems;  
 – the development of an ab-initio theory for the calculation of frequency-dependent Raman spectra of semiconductors, that I am also implementing in the Quantum ESPRESSO code.

Oct 2018-Oct 2020 **Master’s degree in Physics, Sapienza University of Rome (Italy), 110/110 with honors**  
 Thesis advisor: Prof. Francesco Mauri  
 Thesis title: "Giant effective charges in substituted conjugated polymers"  
 – Conjugated polymers, a class of 1D materials, present a peculiar polar response highlighted by anomalously high effective charges. This phenomenon has topological origin and finds its roots in the adiabatic charge transport mechanism of Thouless’ pump.  
 Main topics covered in my Master’s studies are Condensed Matter Physics and Solid State Physics.

Oct 2015- Oct 2018 **Bachelor’s degree in Physics, Sapienza University of Rome (Italy), 110/110 with honors**  
 Thesis title: "Geometric phase in Quantum Mechanics"  
 Thesis advisor: Prof. Andrea Pelissetto

Sep 2010- Jul 2015 **High School Diploma, Liceo Scientifico "B. Rescigno", Roccapiemonte (SA), Italy, 100/100 with honors**

**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](https://europa.eu/europass/levels)

## PRIZES AND AWARDS

- 2023 **Grant for young researchers** "Sapienza" University of Rome  
Funding for research activities granted by Sapienza University of Rome (Sapienza "Avvio alla ricerca" Calls). After going through a review and grading procedure, the project on "Investigation of optical and electromechanical properties of conjugated polymers with quantum and anharmonic effects", submitted in collaboration with a peer PhD candidate, was awarded with the maximum funding for the young researchers' category (4000 euros).
- 2022 **High-Performance Computing (HPC) calls** CINECA  
Computing time granted by the CINECA center, the most powerful supercomputing center for scientific research in Italy, through the ISCRA-C calls. I was the principal investigator of the ECoPol, "Electromechanical properties of Conjugated Polymers" and QuACoPo, "Quantum Anharmonic effects on Conjugated Polymers" projects, granted for a total of more than 200,000 core-hours on the Galileo100 cluster.
- 2020 **PhD scholarships** "Sapienza" University of Rome and SISSA  
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)
- 2020 **Honours Programme for Master's students** "Sapienza" University of Rome  
Mastering activities addressed to the 15 Master's students with the highest GPAs (10% student accepted)
- 2018 **Honours Programme for Bachelor's students** "Sapienza" University of Rome  
Mastering activities addressed to the 30 Bachelor's students with the highest GPAs (10% student accepted)
- 2018 **Tuition fees exemption** "Sapienza" University of Rome  
Scholarship awarded to high-achieving students which guarantees full financial coverage of the tuition fees throughout the Bachelor's degree

## LIST OF PUBLICATIONS

**Giant piezoelectricity driven by Thouless pump in conjugated polymers**

Stefano P. Villani, Marco Campetella, Paolo Barone, Francesco Mauri  
arXiv preprint arXiv:2308.16070. (2023)

## TEACHING AND TUTORING

**Teaching assistant and students' tutor**

- 2021 to 2023 Computational Physics ("Laboratorio di Calcolo", "Laboratorio di Fisica Computazionale I") for Bachelor's students in Physics, Sapienza University of Rome, A.Y. 2021/2022 and 2022/2023.
- 2021 General Physics ("Fisica Generale"), Bachelor's degree in Geology, Sapienza University of Rome, A.Y. 2020/2021.
- 2018 to 2019 Experimental Physics ("Laboratorio di Meccanica", "Laboratorio di Elettromagnetismo e Circuiti", "Laboratorio di Termodinamica"), Sapienza University of Rome, A.Y. 2018/2019 and 2019/2020.

## CONFERENCES, TALKS AND SCHOOLS

- Sep 2023 **CMD30-FisMat2023 - Milan, Italy** Contributed talk  
Joint event of the "Italian national biennial conference on Condensed Matter Physics" (Fis-Mat2023) with the "Biennial conference of the Condensed Matter Division of the European Physical Society" (CMD30). I participated with a contributed talk titled "Topology-induced giant piezoelectricity in conjugated polymers".

- Jul 2023 **SSCHA School 2023 - Donostia/San Sebastian, Spain** Contributed talk  
Summer School on the Calculation of Ionic Quantum and Anharmonic Effects with the Stochastic Self-Consistent Harmonic Approximation (SSCHA). I participated with a contributed talk titled "Strong effects of quantum anharmonicity on the structural and electronic properties of carbyne.
- Jun 2023 **CMT@Brixen 2023 - Bressanone/Brixen, Italy** Attendee  
Meeting of the Condensed Matter Theory (CMT) Italian community
- Jan 2023 **Total Energy 2023 - ICTP, Trieste, Italy** Poster presentation  
21st International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods. I presented a poster with the results of my research on topology-induced giant piezoelectricity in conjugated polymers.
- Aug 2022 **Psi-k conference 2022 - Lausanne, Switzerland** Poster presentation  
6th general conference for the worldwide Psi-k community. I presented a poster with the results of my research on the strong effects of quantum anharmonicity on the structural and polar properties of infinite linear acetylenic carbon chains.
- May 2022 **ML4M 2022 - SISSA, Trieste, Italy** Attendee  
Young Researcher's Workshop on Machine Learning for Materials held at SISSA in Trieste.
- Jul 2021 **QMC School with turboRVB - Virtual/SISSA, Trieste, Italy** Attendee  
Virtual school on ab initio Quantum Monte Carlo simulations with the TurboRVB computational package organized by the SISSA.

## ADDITIONAL INFORMATION

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### Other activities

Mar 2023 - today I currently held the position as representative of the PhD students in the Physics Department Council.

Jan 2022 - today PhD Seminars organizer

The PhD Seminars are events organized every other week by a group of PhD students, of which I am a member, to give the opportunity to fellow PhD students to present their research to the broad community of physics Master's students, PhD students and early post-doctoral researchers in an informal atmosphere.

### Skills

DFT codes CRYSTAL: user

Quantum ESPRESSO: user and developer

Programming languages C, C++, Python, Fortran

Other softwares Matlab,  $\LaTeX$ , Office package