

Assistant Professor, Department of Applied Physics and Applied Mathematics, Columbia University  
200 S.W. Mudd, 500 W. 120th Street, New York, NY 10027, USA  
✉ ms7219@columbia.edu • He/Him

## Education and scientific posts

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**Jan 2025–: Assistant Professor of Applied Physics and Applied Mathematics, Columbia University.**

Research Topics: (i) Quantum transport phenomena, from first principles theories to sustainable technologies;  
(ii) Mesoscopic partial-differential equations for non-diffusive transport of charge, heat, or spin;  
(iii) Design of materials for thermoelectrics, spintronics, and aerospace applications.

**Sep 2021–Dec 2024: Research Fellow, Physics Department (Cavendish Lab), University of Cambridge.**

Research Topics: (i) hybrid crystal-glass transport properties in materials with controlled atomistic disorder;  
(ii) Machine-learning methods for materials simulations.

**Sep 2016–May 2021: PhD in Materials Science and Engineering, EPFL, Switzerland.**

Dissertation: *Thermal transport beyond Fourier, and beyond Boltzmann*, supervised by Prof N. Marzari.

**Sep 2014–Jul 2016: International Master in Physics of Complex Systems, 110/110 with honours.**

Excellence program (admission limited to 20 students) involving SISSA (Trieste), Politecnico di Torino, École Normale Supérieure Cachan (Paris), Universities Paris 6,7,11. Thesis: *Molecular simulation of aqueous electrolytes in nanoporous carbons: blue energy and water desalination*, supervised by Prof M. Salanne.

**Sep 2011–Jul 2014: Bachelor's degree in Physics, University of Trento (Italy), 110/110 with honours.**

Thesis: *Investigation of dispersion and nonlinear effects on the evolution of wave packets*, with Prof G. Garberoglio.

## Fellowships

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**2021-2025:** Patricia Crone Research Fellowship, Gonville & Caius College, University of Cambridge.

**2021-2023:** Postdoc Mobility Fellowship, Swiss National Science Foundation.

## Selected Awards

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**2023:** [Swiss Physical Society award in Computational Physics sponsored by COMSOL](#), for '*contributions to a modern theory of thermal transport in solids*'.

**2022:** [EPFL Doctorate Award](#), issued by the École Polytechnique Fédérale de Lausanne to up to three PhD theses per year, chosen over >400 STEM theses, to recognize research work of '*exceptional quality*'.

**2020:** [Dimitris N. Chorafas Foundation Award](#), issued by the Weizmann Institute of Science (Israel) to '*outstanding doctoral researchers worldwide in selected fields in engineering, medicine and the natural sciences*'. The prize rewarded '*research characterized by its high potential for practical applications*'.

**2017:** [Computational thinking award](#), École Polytechnique Fédérale de Lausanne (Switzerland), first prize at a biennial competition on presenting scientific data in an insightful and visually engaging way.

**2015:** [IDEX Paris-Saclay scholarship](#), awarded by Université Paris-Saclay (France) to "*highly talented international students worldwide to enroll in a prestigious French master's degree*".

**2014:** [University of Trento Merit Award](#), for completing the Bachelor's degree with outstanding GPA.

**2012:** [EU Contest for Young Scientists](#), Bratislava. Intel award, covered all costs to attend ISEF 2013 in Phoenix.

**2011:** Italian national prize for excellence in high school, awarded to top 1% students.

### Awards with supervised students.....

**2024:** Best Poster Award at [CECAM node workshop](#), with PhD student Balazs Pota, *Thermal Conductivity Predictions with Foundation Atomistic Models*.

**2024:** Best Talk Award at [Lennard-Jones Centre Showcase Day](#), with PhD student Kamil Iwanowski, *Bond-network entropy controls thermal conductivity of coordination-disordered solids*.

- 2024:** Best Poster Award at [Lennard-Jones Centre Showcase Day](#), with PhD student Bogdan Rajkov, *Non-diffusive transport phenomena in solids*.
- 2023:** Best Internship Award from École Polytechnique (Paris), with master student Barnabé Ledoux, internship *Phonon-photon interactions from first principles and radiative heat transport*.
- 2023:** [Best Poster Award at the LJC showcase day](#), with student Kamil Iwanowski, internship project *Vibrational and thermal properties of nanoporous-carbon electrodes for supercapacitors*.

## Publications

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Up-to-date publication list and bibliometric indices can be found on [Google Scholar \(click here for link\)](#).

## Invited talks & seminars

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1. **Nov 2024**, Invited seminar, department of physics University of Birmingham, UK.
2. **Nov 2024**, Invited seminar, Laboratoire de Physique et d'Étude des Matériaux, Sorbonne Université, Paris.
3. **Jul 2024**, Talk *Machine learning opens a wonderland for looking through glasses* at [CECAM workshop Machine Learning of First Principles Observables](#), Fritz-Haber Institute, Berlin.
4. **May 2024**, Seminar *From first-principles theories to sustainable technologies* at Columbia University in the City of New York, department of Applied Physics and Applied Mathematics.
5. **Apr 2024**, Talk *Unified formulations of transport in solids: from quantum wave-particle duality to continuum crossovers* at [Workshop Frontiers in Thermal and Electronic Transport in Materials: A Tribute to Nicola Bonini](#), King's College London.
6. **Mar 2024**, Talk *Hybrid crystal-glass heat transport & radiative effects in disordered solids* at the [Spring meeting of the Condensed-Matter Section of the German Physical Society. Focus session Heat Transport at the Nanoscale: Theory meets Experiment](#), Berlin.
7. **Feb 2024**, Seminar *Unified theories of transport in solids: from crystals to glasses, and from diffusion to viscous hydrodynamics* at University of California San Diego, department of physics.
8. **Feb 2024**, Seminar *Hybrid crystal-glass materials, dual wave-particle transport, and applications to energy or information technologies* at University of Oxford, department of materials, Oxford (UK).
9. **Jun 2023**, Talk *Scaling laws of the thermal conductivity of solids: the role of topological, geometrical, and compositional disorder* at the [International Wigner Workshop 2023, Universitat Autònoma de Barcelona](#).
10. **Jan 2023**, Talk *Trends in the thermal conductivity of solids* at the [21st International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods](#), ICTP, Trieste (Italy).
11. **Dec 2022**, Virtual talk *Quantum thermal transport in solids: coherences, disorder, and viscosities* at [CECAM Mixed-Gen event on Theory and numerical simulation of transport processes in condensed matter](#).
12. **Jul 2022**, Talk *Wigner formulation of thermal transport in solids* at [CECAM workshop Quantum Transport Methods and Algorithms: From Particles to Waves Approaches](#), ETH Zurich (CH).
13. **Nov 2021**, Talk *Thermal transport beyond the Ioffe-Regel limit, and resonances in heat hydrodynamics*. [Lennard-Jones Centre, University of Cambridge \(UK\)](#).
14. **Jul 2020**, Virtual talk *Unified theory of thermal transport in crystals and glasses* at the Quantum Matter Institute, University of British Columbia (Canada).
15. **Feb 2020**, Seminar *Thermal transport beyond Fourier, and beyond Boltzmann* at the [Cavendish Laboratory, University of Cambridge \(UK\)](#).

16. Jun 2019, Talk *Unified theory of thermal transport in crystals and glasses & viscous heat hydrodynamics*. Conference on Nanophononics, Bridging Statistical Physics, Molecular Modeling and Experiments. ICTP Trieste.

## Teaching

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University Lecturer.....

2024: Lecturer for the 2nd-year (1B) Natural Sciences undergraduate course *Quantum Physics* at University of Cambridge.

2024: Graduate course *Viscous thermoelectric transport in solids*, Physics Department, condensed matter physics program, University of Cambridge.

2022: Graduate course *Wigner's phase-space formulation of quantum mechanics*, Physics Department, condensed matter physics program, University of Cambridge.

Invited Lectures at Summer Schools.....

2024: Lecturer at *AMaSiS 2024: Applied Mathematics and Simulation for Semiconductor Devices*, Weierstrass Institute Berlin (DE), September 10-15 2024.

2023: Lecturer at *TDEP2023: Finite-temperature and anharmonic response properties of solids in theory and practice*, Linköping University (Sweden), August 21-25 2023.

2023: *International Workshop on Computational Nanotechnology 2023, Universitat Autònoma de Barcelona*. Tutorial *Quantum ESPRESSO: from density-functional theory to dual wave-particle transport*. June 2023.

University teaching assistant.....

2019: Teaching assistant, EPFL master course *Fundamentals of solid-state materials*.

2018: Teaching assistant, EPFL master course *Atomistic and quantum simulations of materials*.

Examination.....

2024: Member of the committee selecting PhD candidates in condensed-matter physics at University of Cambridge.

2023: Member of the committee selecting PhD candidates in condensed-matter physics at University of Cambridge.

2022: Examiner for the first-year PhD exam, University of Cambridge.

2022: Member of the committee selecting PhD candidates in condensed-matter physics at University of Cambridge.

## Software releases

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2022: Implementation in two software of a program that solves the *unified theory of thermal transport in crystals and glasses* [Simoncelli, Marzari, & Mauri, *Nature Physics* **15**, 809 (2019)] and predicts from first principles the thermal conductivity: (i) *phono3py*, (ii) *thermal2* module of Quantum ESPRESSO.

2020: Release in the [documentation of Wolfram Mathematica](#) of an example showcasing the numerical (finite-element) solution of the viscous heat equations derived in [Simoncelli, Marzari, and Cepellotti, *PRX* **10** (2020)].

## Press releases

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- 28.09.2023 G&C College website: *Dr Simoncelli wins Swiss Physical Society Award in Computational Physics*.
- 07.07.2023 NCCR MARVEL website: *Through the glass: predicting the thermal conductivity of glassy insulators from first principles*.
- 05.08.2023 Editorial summary of *Thermal conductivity of glasses: first-principles theory and applications in the Chinese press*: *Glass thermal conductivity challenge: the new Wigner formula*.
- 07.07.2023 NCCR MARVEL website: *Through the glass: predicting the thermal conductivity of glassy insulators from first principles*.
- 15.11.2022 NCCR MARVEL website: *Simoncelli wins 2022 EPFL Doctorate Award for thesis on theory of heat conduction in solids*.
- 01.11.2022 TCM Research Highlights: *Wigner Formulation of Thermal Transport in Solids*.

- 28.10.2020 **NCCR MARVEL website**: [Michele Simoncelli wins the 2020 Chorafas Foundation Award for his contributions to the quantum theory of heat conduction in solids.](#)
- 07.02.2020 **EPFL homepage**: [A novel formulation to explain heat propagation.](#)
- 28.01.2020 **Phys.org**: [Researchers generalize Fourier's 200-year-old heat equation, explaining hydrodynamic heat propagation.](#)
- 14.06.2019 **American Ceramic Society**: [Two materials, one theory—unified thermal transport formula describes heat flow in both crystals and glass.](#)
- 29.05.2019 **Phys.org**: [Researchers introduce novel heat transport theory in quest for efficient thermoelectrics.](#)
- 27.05.2019 **EPFL homepage**: [A novel theory of heat, in the search for efficient thermoelectrics.](#)
- 12.11.2018 **genci.fr**: [Best Use of HPC in Energy award.](#)
- 15.05.2018 **prace-ri.eu**: [Nanoporous Carbon Electrodes Harvest Blue Energy.](#)
- 11.05.2018 **physicsworld.com**: [Nanoporous carbon electrodes harvest blue energy.](#)

## Outreach

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**2022-2023: Gonville & Caius College, University of Cambridge.** Research convenor. Organization of events aiming at promoting interdisciplinary collaborations between academics affiliated with Gonville & Caius College.

**2019:** Member of the jury at the Italian high school scientific contest [I giovani e le scienze](#).

**2018:** Talk *Molecular dynamics in a supercapacitor* at the award ceremony of the [Computational Thinking contest](#), on the use of digital visualization techniques to present scientific data in an engaging way.

**2012:** Presentation of the project *CNC milling machine* at the TV program *Geo scienza* (Rai3, [link YouTube](#)).

## Management, administration, and coaching experiences

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**Oct 2021-: Gonville & Caius College, University of Cambridge.** Fellow & member of the Governing Body. I am voting in the College's general meetings, where academic, financial, and administrative decisions are taken.

**Dec 2021-Jun 2023: Lennard-Jones Centre (LJC), University of Cambridge.** Talk organizer and chair. The LJC brings together researchers from different departments across the University of Cambridge with a common interest in materials and molecular modelling. I co-organized and chaired the talks that took place on a weekly basis.

**Jan 2020-Aug 2021: Sports Universitaires Lausanne.** Cross-country skiing instructor and running coach.

**Jan 2018-Aug 2021: Laboratory of Theory and Simulation of Materials (EPFL).** Assessor and organizer of master projects (interviewed students interested in doing master projects and suggested research topics).

## Contributed talks & posters

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1. **Mar 2023**, Talk *Resonant amplification of hydrodynamic temperature waves in graphite*. APS March Meeting.
2. **Aug 2022**, Talk *Wave-particle duality in heat conduction from Wigner's formalism*. Journées de la Matière Condensée, Lyon (FR).
3. **Aug 2022**, Talk *Heat conduction in complex or disordered solids using the Wigner formulation*. Psi-k conference, Lausanne (CH).
4. **Mar 2022**, Virtual talk *Thermal transport in solids beyond the Ioffe-Regel limit*. APS March Meeting, online.
5. **Oct 2021**, Poster *Quantum thermal transport in solids: coherences, disorder, and viscosities*. Lennard-Jones Centre, University of Cambridge (UK).
6. **Mar 2021**, Virtual talk *Heat transport in ordered and disordered solids within Wigner's phase-space formulation*. APS March Meeting.
7. **Nov 2020**, Talk *Generalization of Fourier's law into viscous heat equations*. International conference on electron-phonon coupling and thermoelectric efficiency. University of the Basque Country (Spain).
8. **Jan 2020**, Talk *A unified theory of thermal transport in crystal and glasses, and a generalization of Fourier's law to heat hydrodynamics*. Conference on Molecular-Scale Charge and Thermal Transport. Engelberg (CH).

9. **Mar 2019**, Talk *Unified theory of thermal transport in crystals and glasses*. APS March Meeting 2019. Boston.
10. **Jan 2019**, Poster *Unified theory of thermal transport in crystals and disordered solids*, 19th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods. ICTP, Trieste (Italy).
11. **Sep 2018**, Poster *Thermal transport in 2D transition metal dichalcogenides within the relaxon picture*, COMDI Conference. Lausanne (Switzerland). **Best poster award**.
12. **Apr 2018**, Talk *Thermal transport in 2D transition metal dichalcogenides*. DPG Conference, Berlin.
13. **Sep 2017**, Poster *Thermal transport in layered and 2D materials within the relaxons picture*, Paris International School on Advanced Computational Materials Science. Université Pierre et Marie Curie (Paris). **Poster award**.