Michele Simoncelli | Curriculum Vitae

Assistant Professor, Department of Applied Physics and Applied Mathematics, Columbia University
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Education and scientific posts

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 nuclear reactors, 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.

01 Sep 2016–26 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

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

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

Selected Awards

2025: Charles Haenny Prize for Physics of '*excellent scientific quality and internationally competitive, while also respectful of humanity and its environment*'.

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.*

Software releases

2025: Coupled BTE module of the phoebe code and SOLver for VIscous ThErmoelectric equations (SOLVITE). This software suite computes thermoelectric transport coefficients from a first-principles solution of the full coupled electron-phonon Boltzmann transport equation, and employs them to parametrize a set of viscous thermoelectric equations, mesoscopic partial-differential equations that are solved using a finite-element solver.

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)].

Invited talks & seminars

1. **Apr 2026**, Invited talk at 2026 MRS Spring Meeting, Honoluli, Hawaii.
2. **Mar 2026**, Invited talk at Global Physics summit, Denver, Colorado.
3. **Sep 2025**, Invited talk at Haenny prize in Physics, Lausanne, Switzerland.
4. **Aug 2025**, Invited talk at the Psi-k Volker Heine Early-Career Investigator (VHECI) Award, Lausanne, Switzerland.
5. **Aug 2025**, Invited talk Thermal Kharkiv Seminar, online.
6. **Jul 2025**, Invited talk, High Frequency Dynamics in Liquids & Glasses (No. 42), 10th IDMRCS, Barcelona, Spain.
7. **Jul 2025**, Invited talk,Fismat 2025 Workshop "Ions in motion: innovative models for heat and charge transport in insulators, Venice (Italy).
8. **Jun 2025**, Invited talk, Thermal Transport at the Nanoscale: June 24-28, 2025, Telluride, USA.
9. **Dec 2024**, Invited seminar, department of physics, University of Trento, Italy.
10. **Nov 2024**, Invited seminar, department of physics, University of Birmingham, UK.
11. **Nov 2024**, Invited seminar, Laboratoire de Physique et d'Etude des Matériaux, Sorbonne Université, Paris.
12. **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.
13. **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.
14. **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.
15. **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.
16. **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.

17. **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).
18. **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.
19. **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).
20. **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.
21. **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).
22. **Nov 2021**, Talk *Thermal transport beyond the Ioffe-Regel limit, and resonances in heat hydrodynamics*. Lennard-Jones Centre, University of Cambridge (UK).
23. **Jul 2020**, Virtual talk *Unified theory of thermal transport in crystals and glasses* at the Quantum Matter Institute, University of British Columbia (Canada).
24. **Feb 2020**, Seminar *Thermal transport beyond Fourier, and beyond Boltzmann* at the Cavendish Laboratory, University of Cambridge (UK).
25. **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.

Management, administration, and coaching experiences

2021-2024: **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.

Teaching

2026: Course for advanced undergraduate and graduate students at Columbia: *Atomic Foundation Models*.

2025: Undergraduate course at Columbia: *Thermodynamics, statistical mechanics, and kinetic theory.*

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

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.

Publications

Up-to-date publication list can be found on Google Scholar: `https://bit.ly/3nPI2B5`

Press releases

- 09.12.2025 **Columbia quantum initiative:** *Columbia Scientists Explain How Atomic Disorder Controls Heat.*
- 04.12.2025 **Columbia apam:** *Michele Simoncelli receives the 2025 Charles Haenny Prize in Physics.*
- 14.07.2025 **Columbia Engineering:** *Hybrid Crystal-Glass Materials from Meteorites Transform Heat Control.*
- 03.12.2024 **G&C College website:** *Dr Simoncelli thanks Caius as he moves to Columbia.*
- 01.10.2024 **matbench discovery:** *Thermal conductivity benchmark metric on the Matbench-discovery platform.*
- 28.09.2023 **G&C College website:** *Dr Simoncelli wins Swiss Physical Society Award in Computational Physics.*
- 07.07.2023 **NCCR MARVEL:** *Through the glass: predicting the thermal conductivity of glassy insulators.*

- 15.11.2022 **NCCR MARVEL:** *Simoncelli wins 2022 EPFL Doctorate Award for thesis on theory of heat conduction.*
- 01.11.2022 **TCM Research Highlights:** *Wigner Formulation of Thermal Transport in Solids.*
- 28.10.2020 **NCCR MARVEL:** *Michele Simoncelli wins the 2020 Chorafas Foundation Award.*
- 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.*
- 14.06.2019 **American Ceramic Society:** *Two materials, one theory—unified thermal transport formula describes heat flow in both crystals and glass.*
- 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.*