

Stefano Baroni

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Present position

2025– Retired **visiting professor** at Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste

Education

1978 Degree *Laurea in Fisica*, University of Pisa (Italy), with honors

Previous positions

1999-2025 **Full professor** of theoretical condensed matter physics at SISSA
 1994-98 **Director**, Centre Européen de Calcul Atomique et Moléculaire (CECAM), then hosted at the École Normale Supérieure de Lyon, France
 1988-99 **Associate professor** at SISSA
 1984-88 **Assistant professor** (*Ricercatore*) at the Department of Theoretical Physics, University of Trieste, Italy
 1979-84 **Postdoc** (*Assistant*) at Institute of Theoretical Physics of the École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Institutional responsibilities

2022– **Co-leader** of the *Materials and molecular sciences* “spoke” (section) of the Italian [National Centre for HPC, Big Data, and Quantum Computing](#).
 2007-10 **Head** of the Condensed Matter Theory Sector (department) at SISSA and **Member** of the SISSA Academic Senate
 2001-08 **Founding director** of the INFM¹ DEMOCRITOS National Simulation Center
 1998-03 **Head** of the Trieste INFM¹ research unit and **Member** of the INFM¹ board of directors

Commissions of trust

2016-17 **Member** of the International Advisory board of the [NFFA](#) EU distributed facility
 2015-16 **Member** of the Physics Panel of the ANVUR-VQR valuation committee of the Italian universities
 2015 **Member** of the Portuguese FCT Science and Engineering panel
 2014-20 **Member** of the PE3 ERC *starting grant* panel
 2012– **Member** of the Scientific Council of the CINECA supercomputing center
 2009-12 **Member** of the CECAM Scientific Advisory Committee
 2005-14 **Member** of the [Eurotech](#) Scientific Advisory Board
 2004-07 **Member** of the SISSA Board of Directors
 2001-06 **Member** of the SISSA valuation committee

Visiting professorships

2013 Laboratoire des Solides Irradiés, École Polytechnique, Palaiseau, France (3 months)
 2012-13 Department of Materials Science, EPFL (6 months)
 2011 CECAM, then hosted at the EPFL (2 months)
 2007 Department of Earth Sciences, University College London, UK (4 months), with a research fellowship of the *Leverhulme Trust*

¹Istituto Nazionale per la Fisica della Materia, now belonging to the Italian CNR
 updated December 23, 2025

2007	School of Physics, University of Sidney, Australia (1 month)
2005	Department of Chemical Engineering and Materials Science, University of Minnesota (1 month)
2004	Laboratoire de Physique des Milieux Condensés, Université Pierre et Marie Curie, Paris, France (1 month)
2002	Chemistry Department, Princeton University (2 months)
1994	Institute for Theoretical Physics, University of California at Santa Barbara (3 months)
1992	Forum Teorico of the INFM ¹ , Scuola Normale Superiore, Pisa, Italy (2 months)
1990-93	Institut Romand de Recherche Numérique sur les Matériaux, EPFL (10 months in total)

Scientific production

SB has authored ≈ 270 scientific publications in peer reviewed scientific journals and conference proceedings, having garnered $\approx 60,000/82,000$ citations (Web of Science/Google Scholar) and earning him an H index of 65/77, as of December 2025.

Invited talks and lectures

SB has given 80+ invited talks and lectures at international scientific meetings, training courses, and scientific institutions over the past 10 years. A complete list of SB's recent invited lectures and talks can be found at <http://talks.baroni.me>.

Scientific profile

SB's scientific interests are at the frontier between condensed-matter theory and simulation, with a penchant for software engineering and high-performance computing: he likes to develop methods to compute properties and simulate processes previously deemed inaccessible to scientific computation, to implement them in high-performance computer codes,¹ and to apply them to problems that are scientifically and technologically relevant. He is largely credited for the introduction of density-functional perturbation theory (DFPT),^{2,3} a methodology that is considered the state of the art for the computation of lattice dynamical properties in solids, including phonon frequencies⁴ and lifetimes.⁵ He has pioneered $\mathcal{O}(N)$ methods in electronic-structure theory⁶ and he has also introduced important innovations in quantum stochastic simulations, including the first application of *Auxiliary-Fields Quantum Monte Carlo* to electronic-structure problems^{7,8} and the introduction of *Reptation Quantum Monte Carlo*,⁹ a method that allows computing with great precision the low-lying spectrum of interacting bosons, with prominent applications to Helium droplets¹⁰ and extensions to interacting fermions.¹¹ Recently, he has successfully extended DFPT so as to encompass electronic excited states through time-dependent density-functional^{12,13} and many-body perturbation theories.^{14,15} He has thoroughly applied these methodological innovations to a number of problems in semiconductor physics, the chemical physics of metal surfaces, and, more recently, molecular and magnetic spectroscopies. Over the past 10 years SB has given important contributions to the theory and numerical simulation of adiabatic heat and charge transport in liquid and disordered systems.^{16–23}

SB's full list of publications is available at his [ORCID profile](#).

Teaching activity

Since 1988 SB is professor of Theoretical Condensed-Matter Physics at SISSA, where he has regularly taught graduate courses in *Quantum Simulations*, *Electronic Structure Theory*, *Transport Theory*, and, in the past, *Atomic Physics* and *Group Theory*.

Mentorship

Stefano Baroni has supervised 36 PhD and 11 Master theses at SISSA, the École Normale Supérieure in Lyon, and the Universities of Trieste, Modena, and Cagliari, many of whom have become internationally recognized scientific leaders. A complete list of former students with links to their theses and info on their present positions, where available, can be found at <http://alumni.baroni.me>.

Community service

SB is the initiator of the [QUANTUM ESPRESSO project](#) and founding director of the [QUANTUM ESPRESSO Foundation](#). He is also the initiator and main inspirer of the very successful [QUANTUM ESPRESSO series of tutorials and electronic-structure schools](#), attended by 2,000+ participants worldwide, in many of which he has acted as one of the organizers and/or lecturers.

Entrepreneurship

SB is founder, shareholder, and Senior Scientific Advisor of [Materys](#), a startup that provides advanced quantum simulation solutions of materials *as a service*.

Honors

SB is a fellow of the American Physical Society (since 2007) and a member of the *Accademia Peloritana dei Pericolanti* in Messina (Italy, since 2005). He is the recipient of the 2026 *Anees Rahman Prize for Computational Physics*, awarded by the American Physical Society.

References

- [1] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. D. Corso, S. Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougousis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, and R. M. Wentzcovitch, *J. Phys. Condens. Matter* **21**, 395502 (19pp) (2009).
- [2] S. Baroni, P. Giannozzi, and A. Testa, *Phys. Rev. Lett.* **58**, 1861 (1987).
- [3] S. Baroni, S. de Gironcoli, A. Dal Corso, and P. Giannozzi, *Rev. Mod. Phys.* **73**, 515 (2001).
- [4] P. Giannozzi, S. De Gironcoli, P. Pavone, and S. Baroni, *Phys. Rev. B* **43**, 7231 (1991).
- [5] A. Debernardi, S. Baroni, and E. Molinari, *Phys. Rev. Lett.* **75**, 1819 (1995).
- [6] S. Baroni and P. Giannozzi, *Europhys. Lett.* **17**, 547 (1992).
- [7] S. Sorella, S. Baroni, R. Car, and M. Parrinello, *Europhys. Lett.* **8**, 663 (1989).
- [8] P. L. Silvestrelli, S. Baroni, and R. Car, *Phys. Rev. Lett.* **71**, 1148 (1993).
- [9] S. Baroni and S. Moroni, *Phys. Rev. Lett.* **82**, 4745 (1999).
- [10] S. Moroni, A. Sarsa, S. Fantoni, K. E. Schmidt, and S. Baroni, *Phys. Rev. Lett.* **90**, 143401 (2003).
- [11] G. Carleo, S. Moroni, F. Becca, and S. Baroni, *Phys. Rev. B* **83**, 1 (2011).
- [12] B. Walker, A. M. Saitta, R. Gebauer, and S. Baroni, *Phys. Rev. Lett.* **96**, 113001 (2006).
- [13] D. Rocca, R. Gebauer, Y. Saad, and S. Baroni, *J. Chem. Phys.* **128**, 154105 (2008).
- [14] P. Umari, G. Stenuit, and S. Baroni, *Phys. Rev. B* **79**, 201104 (2009).
- [15] P. Umari, G. Stenuit, and S. Baroni, *Phys. Rev. B* **81**, 115104 (2010).
- [16] A. Marcolongo, P. Umari, and S. Baroni, *Nat. Phys.* **12**, 80 (2016).
- [17] L. Ercole, A. Marcolongo, and S. Baroni, *Sci. Rep.* **7**, 15835 (2017).
- [18] S. Baroni, R. Bertossa, L. Ercole, F. Grasselli, and A. Marcolongo, “Heat transport in insulators from ab initio Green-Kubo theory,” in *Handbook of Materials Modeling: Applications: Current and Emerging Materials*, edited by W. Andreoni and S. Yip (Springer International Publishing, Cham, 2018) pp. 1–36, 2nd ed., [arXiv:1802.08006 \[cond-mat.stat-mech\]](https://arxiv.org/abs/1802.08006) .
- [19] R. Bertossa, F. Grasselli, L. Ercole, and S. Baroni, *Phys. Rev. Lett.* **122**, 255901 (2019).
- [20] F. Grasselli and S. Baroni, *Nat. Phys.* **15**, 967 (2019).
- [21] L. Isaeva, G. Barbalinardo, D. Donadio, and S. Baroni, *Nat. Commun.* **10**, 3853 (2019).
- [22] F. Grasselli, L. Stixrude, and S. Baroni, *Nat. Commun.* **11**, 3605 (2020).
- [23] P. Pegolo, F. Grasselli, and S. Baroni, *Phys. Rev. X* **10**, 1 (2020).