

Stefano Baroni

ORCID: [0000-0002-3508-6663](https://orcid.org/0000-0002-3508-6663)
 Affiliation: Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste (Italy)
 Birth: August 30, 1955
 Nationality: Italian
 Personal web site: <http://stefano.baroni.me>

Present position

1999- **Full professor** of theoretical condensed matter physics at SISSA

Education

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

Previous positions

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 INF^M¹ DEMOCRITOS National Simulation Center
 1998-03 **Head** of the Trieste INF^M¹ research unit and **Member** of the INF^M¹ board of directors

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*
 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 INF^M¹, 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 230+ scientific publications in peer reviewed scientific journals and conference proceedings, having gathered $\approx 50,000/67,000$ citations (Web of Science/Google Scholar) and earning him

¹Istituto Nazionale per la Fisica della Materia, now belonging to the Italian CNR

an H index of 61/71 as of April 2024.

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://stefano.baroni.me/alumni>.

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).

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. Schlauro, 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).