

Stefano Baroni

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Affiliation: Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste (Italy)
Birth: August 30, 1955
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Present position

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

Education

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

Previous positions

1994-98 **Director**, Centre Européen de Calcul Atomique et Moléculaire (CECAM) 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 the École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Institutional responsibilities

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

Visiting professorships

2013 Laboratoire des Solides Irradiés, École Polytechnique, Palaiseau, France (3 months)
2012-13 Department of Materials Science, EPFL (6 months)
2011 CECAM, EPFL (2 months)
2007 University College London, UK (4 months), awardee of the *Leverhulme Trust*
2007 School of Physics, University of Sidney, Australia (1 months)
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 INFM¹, 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 ≈ 220 scientific publications in peer reviewed scientific journals and conference proceedings, having gathered $\approx 32,000/42,000$ citations (Web of Science/Google Scholar) and earning him an H index of 56/64, as of November 2020. SB's scientific interests are at the frontier between theory and simulation: he likes to invent methods to compute properties and simulate processes previously

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

deemed inaccessible to scientific computation, and to apply them to problems that are scientifically and technologically important. He is largely credited for the introduction of density-functional perturbation theory (DFPT),^{1,2} a methodology that is considered the state of the art for the computation of lattice dynamical properties in solids, including phonon frequencies³ and lifetimes.⁴ He has pioneered $\mathcal{O}(N)$ methods in electronic-structure theory⁵ 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^{6,7} and the introduction of *Reptation Quantum Monte Carlo*,⁸ a method that allows computing with great precision the low-lying spectrum of interacting bosons, with prominent applications to Helium droplets⁹ and extensions to interacting fermions.¹⁰ Recently, he has successfully extended DFPT so as to encompass electronic excited states through time-dependent density-functional^{11,12} and many-body perturbation theories.^{13,14} 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 5 years SB has given important contributions to the theory and numerical simulation of adiabatic heat and charge transport in liquid and disordered systems¹⁵⁻²³.

SB's full list of publications with some bibliometric indices is available at his [Researcher ID page](#).

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*, and, in the past, *Atomic Physics* and *Group Theory*.

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>.

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 more than 1,200 participants worldwide, in many of which he has acted as one of the organizers and/or lecturers.

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).

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