Stefano Baroni

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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 ***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 INFM[1] DEMOCRITOS National Simulation Center

1998-03 **Head** of the Trieste INFM[1] research unit and **Member** of the INFM[1] 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- **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, 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)

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

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 ≈ 210 scientific publications in peer reviewed scientific journals and conference proceedings, having gathered ≈ 22,000/29,000 citations (ISI/google) and earning him an H index of 52/59. SB's scientific interests are at the frontier between theory and simulation: he likes to invent methods to compute properties and simulate processes previously deemed inaccessible to scientific computation, and to apply them to problems of paramount scientific and technological importance. 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 frequencies[3] and lifetimes,[4] and that is instrumental in the recent upsurge of the application of the Boltzmann's transport equation to heat conduction in materials.[5] He has pioneered $\mathcal{O}(N)$ methods in electronic-structure theory[6] 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 droplets[10] 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 spectroscopy. Of direct relevance to the present project is SB's recent work on thermal transport.[16–18]

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. SB's recent work on thermal transport[16–18] has attracted a certain attention and earned him a number of invitations at important international meetings, including the 2017 March Meeting of the APS and the XXIX IUPAP Conference on Computational Physics.

A complete list of SB's recent invited lectures and talks can be found at http://talks.baroni.me.

Mentorship

Stefano Baroni has supervised 29 PhD and 8 Master thesis at SISSA, the École Normale Supérieure in Lyon, and the Universities of Trieste, Modena, and Cagliari, and 25 postdoctoral fellows at SISSA, CECAM, and INFM/CNR, many of whom have become internationally recognized scientific leaders.

A complete list of students and postdocs with links to their theses and info on their present position, where available, can be found at the SB's students and SB's postdocs pages.

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 that 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).

Ten-years track record

Key numbers (2008-)

Publications:	43
Citations:	7500+
10-years H-Index:	17
Invited talks:	80+

10 main publications since 2008 (not necessarily the most cited ones)

10 L Ercole, A. Marcolongo, and S. Baroni, *Accurate thermal conductuvities from optibally short molecular dynamics simulations*, Sci. Rep. **7**, 15835 (2017);

9 A. Marcolongo, P. Umari, and S. Baroni, *Microscopic theory and quantum simulation of atomic heat transport*, Nature **12**, 80 (2016) **(12 cites)**;

8 L. Ercole, A. Marcolongo, P. Umari, and S. Baroni, *Gauge Invariance of Thermal Transport Coefficients*, J. Low. Temp. Phys. **185**, 79 (2016);

7 *Dielectric and Thermal Effects on the Optical Properties of Natural Dyes: A Case Study on Solvated Cyanin*, J. Am. Chem. Soc. **133**, 15425 (2011) **(28 cites)**;

6 P. Umari, G. Stenuit, and S. Baroni, *GW quasiparticle spectra from occupied states only*, Phys. Rev. B **81**, 115104 (2010) **(97 cites)**;

5 S. Baroni, P. Giannozzi, and E. Isaev, *Density-Functional Perturbation Theory for Quasi-Harmonic Calculations*, Rev. Mineral. Geochem. **71**, 39-57 (2010) **(112 cites)**;

4 P. Umari, G. Stenuit, and S. Baroni, *Optimal representation of the polarization propagator for large-scale GW calculations*, Phys. Rev. B **79**, 201104 (2009) **(64 cites)**;

3 P. Giannozzi, S. Baroni *et al.*, *QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials*, J. Phys. Condens. Matter, **21**, 395502 (2009) **(7263 cites)**;

2 D. Rocca, R. Gebauer, F. De Angelis, M.K. Nazeeruddin, and S. Baroni, *Time-dependent density functional theory study of squaraine dye-sensitized solar cells*, Chem. Phys. Lett. **475**, 49 (2009). **(65 cites)**;

1 D. Rocca, R. Gebauer, Y. Saad, and S. Baroni, *Turbo charging time-dependent density-functional theory with Lanczos chains*, J. Chem. Phys. **128**, 154105 (2008) **(119 cites)**.

10 main invited talks and lectures

10 Keynote talk given at the XXIX IUPAP Conference on Computational Physics, Paris, July 9-13, 2017: *Car and Parrinello meet Green and Kubo: simulating atomic heat transport from equilibrium ab-initio molecular dynamics*;

9 Talk to be given at the March Meeting of American Physical Society, New Orleans, LA, March 13-17, 2017: *Car and Parrinello meet Green and Kubo: simulating atomic heat transport from equilibrium ab-initio molecular dynamics*;

8 Greater Boston area theoretical chemistry lecture, given at Harvard University, Cambridge MA, October 24, 2013: *Ab initio colors*;

7 Talk given at the 15th Asian Workshop on First-Principles Electronic Structure Calculations, November 5-7, 2012, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei: *Modeling the color of natural dyes*;

6 Plenary talk given at the Ψ_k 2010 Conference, Berlin, September 12-16, 2010: *Powering computational spectroscopy into the hundred-of-atoms size range and beyond*;

5 Talk given at the Fall meeting of the American Geophysical Union, San Francisco CA, December 14-18, 2009: *Computational spectroscopy with QUANTUM ESPRESSO*;

4 Talk given at the Gordon Research Conference on Time-dependent density-functional theory, Colby College, New London NH, July 5–20, 2009: *Harnessing molecular excited states with Lanczos chains*;

3 Plenary talk given at XIX IUPAP Conference on Computational Physics, Brussels, September 5-8, 2007: *Density-functional perturbation theory goes time-dependent*;

2 Talk given at the Gordon Research Conference on Time-dependent density-functional theory, Colby College, Maine, July 15-20, 2007: *Turbocharging time-dependent density-functional theory with Lanczos chains*;

1 Talk given at the March Meeting of the American Physical Society, Baltimore MD, March 13-17, 2006: *Turbocharging time-dependent density-functional theory with Lanczos chains.*

New scientific interests and research lines

Among the new scientific interests nurtured by SB in the past 10 years, some of the most relevant are:

- **Electronic excited states and molecular spectroscopies.** Building on our consolidated and broadly recognized experience in density-functional perturbation theory, we have developed a novel approach to time-dependent density-functional perturbation theory and many-body perturbation theory that allows computing the electronic excited states of complex molecular and nano-structured systems without making reference to their virtual orbitals (Refs. 2, 3, 5, and 7 above);
- **Industrial research.** Building on the above developments, we have undertaken a program of applied research on the color optical properties of natural dyes (see Ref. 8 above) that has allowed SISSA to sign the most important contract of industrial research ever (see Appendix). We are now successfully working with Mars Inc. to find natural alternatives to the artificial colorants that they currently employ to manufacture some of their confectionery. Many of the important results already achieved are still subject to a non-disclosure agreement and have not yet been published;
- **Thermal transport.** The subject of the present proposal (see Refs. 1 and 2 above).

Appendix: Funding ID

On-going grants

project title	period	funding source	amount (euros)	role of the PI	relation to current ERC proposal
CHROMA	2013-15	Mars Inc.	370,000	PI	none
CHROMA	2016-18	Mars Inc.	280,000	PI	none
MAX	2015-18	EU eINFRA-2015	4,068,864	co-PI and WP leader	will provide advanced IT competences

References

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[2] S. Baroni, S. de Gironcoli, A. Dal Corso, and P. Giannozzi, Rev. Mod. Phys. **73**, 515 (2001).
[3] P. Giannozzi, S. De Gironcoli, P. Pavone, and S. Baroni, Phys. Rev. B **43**, 7231 (1991).
[4] A. Debernardi, S. Baroni, and E. Molinari, Phys. Rev. Lett. **75**, 1819 (1995).
[5] J. Zhou, B. Liao, and G. Chen, Semicond. Sci. Technol. **31**, 043001 (2016).
[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, Nature Phys. **12**, 80 (2016).
[17] L. Ercole, A. Marcolongo, P. Umari, and S. Baroni, J. Low Temp. Phys. **185**, 79 (2016).
[18] L. Ercole, A. Marcolongo, and S. Baroni, "Clean thermal conductivities from dusty numerical simulations," (2017), arXiv:1706.01381 .