

# Stefano Baroni

Professor of Theoretical Condensed Matter Physics,  
Scuola Internazionale Superiore di Studi Avanzati



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## EDUCATION

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

## POSITIONS HELD

- 2007-11 Head of the *Condensed Matter Theory* sector (department) at the *Scuola Internazionale Superiore di Studi Avanzati* (SISSA), Trieste, Italy (<http://www.sissa.it>).
- 2002-08 Founding director of the *DEMOCRITOS* National Simulation Center of the Italian *Istituto Nazionale per la Fisica della Materia* (INFN), Trieste, Italy, now part of the *Istituto dell'Officina dei Materiali* of the Italian CNR .
- 1999- Full professor (*Professore ordinario*) of theoretical condensed matter physics at SISSA.
- 1994-98 Director, *Centre Européen de Calcul Atomique et Moléculaire* (CECAM) at the *Ecole Normale Supérieure de Lyon*, France ([www.cecarn.fr](http://www.cecarn.fr)).
- 1988-99 Associate professor (*Professore Associato*) at SISSA.
- 1984-88 Assistant professor (*Ricercatore*) at the Department of Theoretical Physics, University of Trieste, Italy.
- 1980-84 Postdoc (*Assistant*) at the *Laboratoire de Physique Théorique* (LPT) of the *Ecole Polytechnique Fédérale de Lausanne* (EPFL), Switzerland.
- 1979-80 Junior visiting scientist at the LPT-EPFL, Lausanne, Switzerland, with a fellowship of the Italian *Consiglio Nazionale delle Ricerche* (CNR).

## INVITATIONS TO OTHER SCIENTIFIC INSTITUTIONS

- 2013 Visiting professor, *Laboratoire des Solides Irradiés*, Ecole Polytechnique, Palaiseau, France (April to June).
- 2012-3 Visiting Professor, Department of Materials Science, Ecole Polytechnique Fédérale de Lausanne, Switzerland (October to March).
- 2011 Visiting scholar, CECAM, Ecole Polytechnique Fédérale de Lausanne, Switzerland (July and September).
- 2009 Visiting scholar, School of Physics, University of Sidney, Australia (March).

- 2007 *Leverhulme* visiting professor at the University College London, London, UK (four months in Spring and Autumn).
- 2007 Visiting professor, School of Physics, University of Sidney, Australia (March).
- 2005 Visiting professor at the Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis (July).
- 2004 Visiting professor at the *Laboratoire de Physique des Milieux Condensés, Université Pierre et Marie Curie*, Paris, France (June).
- 2002 Visiting professor at the Chemistry Department of the Princeton University (June and August).
- 1994 Visiting scientist at the Institute for Theoretical Physics, University of California at Santa Barbara (April-June).
- 1993 Visiting professor at the *Institut Romand de Recherche Numérique en Physique des Matériaux* (IRRMA), Lausanne, Switzerland (January-March).
- 1992 Visiting professor at *Forum Teorico* of the INFN, Scuola Normale Superiore, Pisa, Italy (November-December).
- 1992 Visiting professor at IRRMA, Lausanne, Switzerland (May-July).
- 1991 Visiting professor at IRRMA, Lausanne, Switzerland (May-July).
- 1990 Visiting professor at IRRMA, Lausanne, Switzerland (February).

## FIELDS OF RESEARCH

- Numerical simulation and modeling in physics, chemistry, and materials science
- Electronic structure and chemical reactivity of metal surfaces
- Lattice-dynamical properties of materials
- Density functional theory
- Quantum simulations of interacting fermions and bosons (particularly He droplets)
- Algorithms and methods for large-scale electronic-structure calculations
- Scientific software engineering

## SCIENTIFIC PRODUCTION

Stefano Baroni is the author of more than 200 scientific papers published in international journals and refereed conference proceedings (182 on ISI: 4 *renowned*, 500+ quotes; 1 *famous*, 250-499 quotes; 16 *very well know*, 100-249 quotes. These papers have been cited 10,000+ times in the international literature (H45, source: ISI, February 2013). Among SB's papers, the most significant include:

1. P. Giannozzi, S. Baroni et al., *Quantum ESPRESSO: a modular and open-source software project for quantum simulations of materials*, J. Phys. Condensed Matter **21**, 395502 (2009).
2. B. Walker, A.M. Saitta, R. Gebauer, and S. Baroni, *Efficient approach to time-dependent density-functional perturbation theory for optical spectroscopy*, Phys. Rev. Lett. **96**, 113001 (2006).

3. A. Kokalj, N. Bonini, S. de Gironcoli, C. Sbraccia, G. Fratesi, and S. Baroni, *Methane Dehydrogenation on Rh@Cu(111): A First-Principles Study of a Model Catalyst*, J. Am. Chem. Soc. **128**, 12448 (2006).
4. S. Moroni, A. Sarsa, S. Fantoni, K.E. Schmidt, and S. Baroni, *Structure, rotational dynamics, and superfluidity of small OCS-doped He clusters*, Phys. Rev. Lett. **90**, 143401 (2003).
5. S. Baroni, S. de Gironcoli, A. Dal Corso, and P. Giannozzi, *Phonons and related properties of extended systems from density-functional perturbation theory*, Rev. Mod. Phys. **73**, 515 (2001).
6. S. Baroni and S. Moroni, *Reptation quantum Monte Carlo: a method for unbiased ground-state averages and imaginary-time correlations*, Phys. Rev. Lett. **82**, 4745 (1999).
7. A. Debernardi, S. Baroni, and E. Molinari, *Anharmonic phonon lifetimes in semiconductors from density-functional perturbation theory*, Phys. Rev. Lett. **75**, 1819 (1995).
8. S. Baroni and P. Giannozzi, *Towards very large-scale electronic-structure calculations*, Europhys. Lett. **17**, 547 (1992).
9. A. Baldereschi, S. Baroni, and R. Resta, *Band offsets in lattice-matched heterojunctions: a model and first-principles calculations for GaAs/AlAs*, Phys. Rev. Lett. **61**, 734 (1988).
10. S. Baroni, P. Giannozzi, and A. Testa, *Green's Function approach to linear response in solids*, Phys. Rev. Lett. **58** 1861 (1987).

Stefano Baroni is the coordinator of the development team of the Quantum ESPRESSO distribution of codes for the simulation of matter at the nanoscale (<http://www.quantum-espresso.org>).

## TEACHING

Stefano Baroni is presently supervising 4 PhD thesis at SISSA. In the past, he has been the supervisor of 19 PhD thesis and of 7 undergraduate thesis at SISSA, at the *Ecole Normale Supérieure de Lyon*, and at the Universities of Trieste, Udine, Cagliari, Modena, and Roma *La Sapienza*. His teaching duties have included so far:

- 1979-88      Teaching assistant at EPFL (until 1984) and University of Trieste (from 1984).
- 1987-        Teacher of graduate courses at SISSA on electronic-structure theory and computer simulations.
- 2002        Teacher of a course on Monte Carlo methods at the University of Udine.

Stefano Baroni has organized or co-organized a number of training courses in computer simulations for young researchers from developed as well as developing countries, in the fields of electronic-structure methods (including hands-on tutorials on the Quantum ESPRESSO package) and quantum Monte Carlo methods.

## OTHER PROFESSIONAL ACTIVITIES

- Referee of several research funding agencies, including the US NSF and the Italian *Comitato dei Garanti* and CIVR.
- Former member of the board of directors of SISSA.
- Former member of the SISSA Internal Valuation Committee.
- Former member of the Board of Directors of the *Istituto Nazionale per la Fisica della Materia* (INFN) and director of the INFN Trieste research unit.

- Former member of the National Scientific Panel of the Theory Section of the INFM.
- Former member of the National Panel for Supercomputing Applications of the INFM (*Iniziativa Trasversale Calcolo Parallelo*), 1995-1998.
- Organizer of several professional meetings at CECAM (France), ICTP (Italy), at the Centro Stefano Franscini (Switzerland), run by the Federal Institute of Technology of Zürich, and of symposia at the annual meeting of the Italian INFM.
- Referee of several scientific journals, including the *Physical Review (B and Letters)*, the *Journal of the American Chemical Society*, the *Journal of Chemical Physics*, and others.
- Member of the Scientific Advisory Committee of the *EuroTech* company (Amaro, UD, Italy).
- Member of the Scientific Advisory Board of the *Centre Européen de Calcul Atomique et Moléculaire, Ecole Polytechnique Fédérale de Lausanne*.

## HONORS

Stefano Baroni is a fellow of the *American Physical Society* and a member of the *Accademia Peloritana dei Pericolanti* in Messina (Italy).