

PRESS RELEASE

The World's Highest Honor in Computational Physics Awarded to Stefano Baroni

The SISSA professor receives the 2026 Rahman Prize, the most prestigious international recognition for those who harness the power of supercomputers to uncover new laws of nature and apply them to cutting-edge technologies.



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The American Physical Society (APS) – the world's largest organization of physicists – has awarded the **2026 Aneesur Rahman Prize for Computational Physics** to **Stefano Baroni**, Professor of Condensed Matter Physics at the Scuola Internazionale Superiore di Studi Avanzati (SISSA) and research associate at the Consiglio Nazionale delle Ricerche – Istituto Officina dei Materiali (CNR–IOM). The prize is regarded as the most prestigious international recognition in the field, awarded for outstanding achievements in computational physics.

The **official citation** recognizes his “seminal contributions to the development of first-principles methods for studying the electronic and thermal properties of condensed systems, and for the development and dissemination of open-source software for electronic-structure calculations, now widely adopted.”



A Professor of Theoretical Condensed Matter Physics at SISSA since 1988, over the course of his career Stefano Baroni has made decisive contributions to tools that are now a shared asset of the entire computational materials physics community. From 1994 to 1998, he served as Director of the Centre Européen de Calcul Atomique et Moléculaire (CECAM), then part of the École Normale Supérieure de Lyon. In 2002, he founded at SISSA the National Center for Numerical Simulation “DEMOCRITOS”, now part of the CNR’s Istituto Officina dei Materiali. Since 2022, he has been co-leader of the “Materials and Molecular Sciences” spoke of ICSC – Centro Nazionale di Ricerca in HPC, Big Data e Quantum Computing, one of the five national centres established under Italy’s PNRR to advance frontier research and innovation. He is also a founding partner of Materys, a SISSA spinoff company providing high-performance cloud computing services.

“Like many recognitions that come later in life, this one is — if not above all — a tribute to the colleagues, and to the students, who made my work possible,” Baroni remarks. “The citation recalls three milestones of my career. The first dates back to the late 1980s when, as a young professor at SISSA, together with Paolo Giannozzi, we developed a method that later became widely used to calculate the dynamical and dielectric properties of solids. The second, in the last decade, concerns the development of a new theory of thermal conduction in condensed matter, made possible thanks to the ingenuity of some of the best students I had the pleasure to mentor at SISSA. Throughout my career, the third — only seemingly less noble, yet equally demanding and impactful — has been the creation, development, and promotion of the Quantum ESPRESSO software, now considered a standard tool for quantum materials simulations, whose development Paolo has long been leading and curating. To all of them goes my deepest and most affectionate gratitude for accompanying and supporting me.”

Underlining the significance of these achievements are the words of **Roberto Car**, Professor at Princeton University, one of the foremost international authorities in the field and, together with Michele Parrinello, creator of the renowned Car–Parrinello quantum simulation method for materials, developed at SISSA in the second half of the 1980s.

“This is a long-overdue recognition of Stefano Baroni’s important contributions to the computational physics of matter. These contributions include an innovative approach to calculating the response of electrons to small displacements of atoms from their equilibrium positions. This approach enabled Stefano and collaborators to predict with remarkable accuracy — starting from the laws of quantum mechanics — the vibrational spectra of crystalline solids as well as phonon–phonon and phonon–electron couplings, crucial for the theory of

superconductivity and thermal and electrical transport. Notably, in the 2010s this approach was successfully extended to treat electronic and magnetic excitations in molecules and extended systems. More recently, Baroni has made a fundamental contribution to the theory of thermal transport by discovering the invariance law that explains why different definitions of heat flux lead to the same thermal conductivity in numerical simulations. Finally, I would like to highlight the **Quantum ESPRESSO** computational platform, of which Stefano was the initiator and main proponent, for first-principles calculations of materials properties — i.e., starting solely from the laws of quantum mechanics. Quantum ESPRESSO is one of the most widely used codes by the large community of physicists, chemists, and engineers studying the microscopic properties of materials. An essential aspect of Quantum ESPRESSO is its open-software nature, which gives users free access and allows them to be, at the same time, users and developers of improvements and new functionalities.”

Named after molecular dynamics pioneer Aneesur Rahman, the Rahman Prize recognizes each year contributions that reshape the practice of computational physics. As already noted in the motivation for his election as an APS Fellow in 2006, Baroni has uniquely bridged the gap between theoretical innovation and practical implementation, creating powerful formalisms and transforming them into tools the community can concretely use. The awarding of this prize reaffirms the value of research that combines theoretical elegance, algorithmic application, and the creation and open sharing of high-quality scientific software.

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