CV – Vincenzo Barone

Brief profile

Vincenzo Barone is an internationally recognized theoretical and computational chemist, with long-standing experience in scientific research, academic leadership, and research evaluation at national and European level. His activity combines methodological developments, interdisciplinary applications, and sustained engagement in research governance, assessment, and policy-related roles. He has held senior academic and institutional positions, coordinated large research programmes, and served on numerous evaluation panels and advisory boards.

Scientific Activity: General Philosophy and Results

The main research interests are related to a theoretical microscopic approach for the study of structural, dynamic, electronic and spectroscopic properties of complex systems (materials, nanostructures, biomolecules, soft matter), as well as of their reactivity. Such an approach is based on the development of integrated tools for the accurate description of physico-chemical processes in condensed phases, including advanced electronic structure models within density functional theory, mixed discrete–continuum descriptions of solute–solvent interactions, and the inclusion of nuclear motion effects ranging from vibrational averaging to quantum and classical dynamics.

Attention has been devoted to achieving computational accuracies comparable to experimental data, while preserving interpretability in terms of basic chemical–physical models and general rules. The focus on realistic systems has naturally led to multiscale approaches, integrating different theoretical models suitable for distinct spatial and temporal scales into coherent and comprehensive descriptions. This research strategy, located at the interface of theoretical and computational chemistry, has aimed at developing integrated and cost-effective computational tools, often supported by long-standing collaborations with leading experimental groups and by a continuous effort to make theoretical developments broadly accessible.

The most significant research fields include density functional theory, solvation theory, and computational spectroscopy. This methodological framework has been employed to describe a wide range of systems and processes, particularly those governed by the interplay between local phenomena and long-range intra- and intermolecular interactions. Space- and time-multiscale approaches have been central to this research philosophy, leading to integrated descriptions of increasing reliability and to the long-term goal of developing and validating virtual instruments for molecular sciences.

Scientific activity and research leadership in theoretical and computational chemistry are evidenced by more than 900 publications in international journals, over 60,000 citations, and an h-index of 105, with 11 papers cited more than 1,000 times. Since 2009, Barone has been included among the ISI Highly Cited Researchers in Chemistry. His research activity has attracted substantial competitive funding from national and European sources and has been acknowledged by several national and international distinctions (Sacconi, Pisani, Bonino and Avogadro Medals, and the Franco-Italien Prize). He is Fellow of the Royal Society of Chemistry, the International Academy of Quantum Molecular Sciences, the European Academy of Sciences, and the Accademia dei Lincei.

Management: Experience and Projects

He has directed one of the leading research groups in the field of theoretical and computational chemistry, including researchers from the Scuola Normale Superiore, the CNR (National Research Council), and the INSTM consortium. A significant component of the group's activity has concerned high-resolution 3D technologies and Cave Automatic Virtual Environments, enabling interactive manipulation of virtual objects across scales ranging from the cosmological to the molecular level. These approaches have also fostered interdisciplinary interactions between the hard sciences and the humanities, with applications to cultural heritage, including archaeological reconstruction, integration of diagnostic data on artworks, and virtual restoration.

Since his appointment at the Scuola Normale Superiore in 2009, a sustained effort has been devoted to strengthening the role of chemistry within the scientific and educational mission of the institution. The increased visibility and impact of chemical disciplines are reflected in his election in 2015 as Dean of the Classe di Scienze Matematiche e Naturali of the Scuola Normale Superiore.
He was the principal proponent and Chair of the Management Committee of the COST Action CM1002 (CODECS), an interdisciplinary project funded within the Chemistry and Molecular Sciences and Technology COST Domain (2010–2014), involving 21 countries and more than 50 research institutions. The action promoted scientific exchange and networking within the European community active in computational spectroscopy.
Another major responsibility has been the coordination of the Chemistry Ph.D. programme at the Scuola Normale Superiore since 2009. In 2014 the programme was extensively restructured and refocused on the development and validation of advanced theoretical and computational methods, with applications spanning astrochemistry, cultural heritage, nanosciences, and life sciences. He has supervised more than 35 Ph.D. students and over 25 postdoctoral researchers, many of whom have subsequently pursued successful academic or industrial careers.
His research activity has consistently attracted competitive funding from public and private institutions and has generated several initiatives with direct implications for technology transfer. Representative examples include projects devoted to cultural heritage restoration and to the development of advanced polymeric materials for smart applications.
A strong ability to design and manage inclusive scientific platforms is evidenced by numerous national and international initiatives, including the direction of a CECAM node at the Scuola Normale Superiore (since 2011), the leadership of the COST Action CODECS, and the organization of the long-standing Winter Modelling conference series.
Management activities aimed at promoting chemistry at the national and international level are further documented by his roles within the Italian Chemical Society, including coordination of the Interdivisional Group on Computational Chemistry, chairmanship of the Division of Chemical Physics, and presidency of the Society (2011–2013). In this capacity, he coordinated initiatives connected with the International Year of Chemistry 2011.
He served as Director of the Institute for Physical-Chemical Processes (IPCF–CNR), one of the largest CNR institutes, characterized by a strong interdisciplinary profile. He later became Director of the DREAMS centre at the Scuola Normale Superiore, integrating high-performance computing and advanced virtual-reality facilities, including large-scale HPC infrastructures hosted at the Avogadro data centre.
Between 2016 and 2019, a substantial part of his activity was devoted to the direction of the Scuola Normale Superiore, with particular emphasis on strengthening international collaborations, partnerships, and the overall research and training offer.
Then, he has been the coordinator of the PhD program in Astrochemistry between 2019 and 2021 and then of the joint MOSES PhD program between SNS and SSM until his retirement on 1/11/ 2023.

Recent Scientific Activity (2020-present)

The period starting in 2020 was significantly affected by the COVID-19 pandemic, which imposed a temporary and forced reduction of on-site scientific and organizational activities. Despite these constraints, research activity was maintained and progressively intensified in the following years.
In 2022 and 2023, while still in service at the Scuola Normale Superiore, Barone actively contributed to the relaunch of scientific interactions within the theoretical and computational chemistry community by organizing major meetings, including the annual Winter Modelling conference, two editions of the Summer Modelling workshop, and the National Conference of the Division of Theoretical and Computational Chemistry of the Italian Chemical Society. In the same period, he resumed the scientific direction of the SMART laboratory at the Scuola Normale Superiore, promoting research activities focused on advanced modelling and spectroscopy.

Following his retirement at the end of 2023, Barone continued his scientific activity as Research Collaborator at INSTM, leading a small and highly motivated group of young researchers. This phase has been characterized by strong scientific productivity and by the consolidation of research lines aimed at extending highly accurate computational methods to medium- and large-size molecular systems. In 2025 alone, 25 scientific papers were published, and his h-index has increased to 105.
Recent work has primarily focused on the extension of accurate and cost-effective composite quantum-chemical schemes to complex molecular systems, with applications to high-resolution rotational and vibrational spectroscopy, semiexperimental structure determination, reactive intermediates, and molecular systems of astrochemical and biochemical relevance.

Evaluation Activity: Previous Experience and Perspectives

Barone has extensive experience in the evaluation of research projects at both national and international level. He has served on numerous Ph.D. committees across Europe and, in 2009, was a member of the Board of Trustees for the evaluation of the Italian PRIN projects funded by MIUR. In 2011, he was member of the Evaluation Committee for research projects at the University of Turin.
He has acted as scientific project evaluator for major national funding agencies, including the U.S. National Science Foundation (NSF), the Austrian FWF, the French ANR, and the Belgian FNRS. He has also participated in self-assessment and advisory activities for academic institutions, including the Chemistry Department of CNRS (France) and the Graduate School of Padua.
He is a member of the Advisory Boards of *Theoretical Chemistry Accounts (since 2005)*, *Journal of Computational Chemistry (since 2007)*, *Physical Chemistry Chemical Physics (since 2011), Spectrochimica Acta A (since 2011), and ChemPhysChem (since 2013)*,
Barone has taken part in numerous national committees for comparative evaluations and recruitment procedures within Italian universities (Physical Chemistry, CHIM/02) and the National Research Council (CNR). In these roles, he has consistently promoted the adoption of transparent evaluation criteria based on internationally recognized indicators, such as impact factors and h-indexes, an approach that has since become widely accepted and reflected in national regulations.
From 2012 to 2014, he served as President of the Chemistry Panel of the National Agency for Research Evaluation (ANVUR), overseeing the evaluation of Italian universities and research institutions and contributing to the definition of general assessment criteria. In 2022, he was appointed coordinator of the evaluation panel for Italian Research Projects (PRIN) across all PE sectors.

Supervision and Mentoring

Barone has extensive experience in the supervision of graduate students and postdoctoral researchers. Between 2008 and 2023, at the Scuola Normale Superiore, he supervised 54 postdoctoral fellows, 35 Ph.D. students, and 30 undergraduate students. In the period 1982–2008, at the University of Naples Federico II, he supervised 25 postdoctoral fellows, 20 Ph.D. students, and 18 undergraduate students. Many of the researchers supervised over the years, including several female scientists, have gone on to successful academic and research careers. Former group members now holding academic positions include Carlo Adamo (Full Professor, Chimie ParisTech), Maurizio Cossi (Associate Professor, University of Eastern Piedmont), Roberto Improta (Senior Research Scientist, CNR), Julien Bloino (Associate Professor, Scuola Normale Superiore), and Nadia Rega (Associate Professor, University of Naples Federico II). Other former group members have pursued research careers in industry, including Giovanni Scalmani (Gaussian, Inc.).

Concluding remarks

Overall, Barone's scientific career combines sustained methodological contributions, interdisciplinary applications, and long-standing experience in research evaluation, academic governance, and mentoring. Alongside continued scientific activity, particular emphasis has been placed on promoting rigorous, transparent, and internationally benchmarked assessment practices, as well as on the training of young researchers within inclusive and high-level research environments.