Prof. Vincenzo Barone, FRSC
Work address
Scuola Normale Superiore
Piazza dei Cavalieri 7
56126 Pisa, Italy
Tel: +39 050 509134
Fax: +39 050 563513
Mob. +39 3316267214
e-mail: vincenzo.barone@sns.it

Summary

This document starts with a section on key features (including main achievements and language skills) and bibliometric data. A short CV comes next, complete of full personal data, brief reviews of scientific activity, management experiences (with special reference to national and international research and academic Institutions) and evaluation activity (concerning both national and international contexts). Finally, the general principles are outlined, which have been shaping Barone's career, with an emphasis on the strong link between frontier research and technological transfer, as one of the most relevant means to keep moving towards our future while remaining competitive.

Index

Key Features

2018 Premio Roma Urbs Universalis, Associazione Ostia Cultura
2017 Philosophiæ Doctor honoris causa in Chemical Sciences by Università di Napoli Federico II
Premio 100 Eccellenze Italiane, RD Editore
Premio Life Gates, Associazione culturale admARTE
Director of the Scuola Normale Superiore
2016 Dean of Classe di Scienze Matematiche e Naturali Scuola Normale Superiore (2015-2017)
2015 Recipient of the *Gian Battista Bonino* medal
Recipient of the *Cesare Pisani* medal
2014 Coordinator of the PhD program: *Methods and Models for Molecular Sciences*
Recipient of Ideas ERC Advanced Grant (DREAMS)
2013 Fellow of *Accademia dei Lincei*
Director of DREAMSLab Centre of the Scuola Normale Superiore
Fellow of *European Academy of Sciences*
2012 Appointed Member of the National Committee of Research Guarantors (CNGR)
President of the Chemistry Panel, National Agency for Research Evaluation (ANVUR)
President of *Italian Chemical Society* (SCI) for the period 2011-2013
2011 Member of the Editorial Board of *Spectrochimica Acta A*
Member of the Advisory Editorial Board of *Open Chemistry*
Fellow of *Academy of Sciences of Bologna*
Director of *CECAM* node at Scuola Normale Superiore
Chair of CM1002 - *CODECS* COST Action (2010-2014)
2010 President of the Computer Center, Scuola Normale Superiore (CEIC)
Coordinator of the Pisa Unit, TO61 Project, National Institute for Nuclear Physics (INFN)
Coordinator of M3-Village network, National Consortium for Material Sciences (INSTM)
Full Professor of Theoretical and Computational Chemistry, Scuola Normale Superiore
2009 Thomson-Reuters ISI *Highly Cited Researcher*
Recipient of the *Luigi Sacconi* medal
Fellow of Royal Society of Chemistry (*FRSC*)
National Coordinator of CNR Project 7 (Computational Modelling)
Member of the Scientific Board of the SCoPE Data Centre (Naples)
Member of the Editorial Board of *Physical Chemistry Chemical Physics*
Director of the *CNR-IPCF* Institute
2008 Fellow of the International Academy of Quantum Molecular Sciences (IAQMS)
Member of the Scientific Council of the Chemistry Department of CNRS, France (2008-2012)
President of the *Chemical Physics Division*, Italian Chemical Society (2007-2009)
2007 Member of the Editorial Board of *Journal of Computational Chemistry*
Coordinator of the *Computational Chemistry* Group, Italian Chemical Society (2005-2007)
2005 Member of the Editorial Board of *Theoretical Chemistry Accounts*
2000 Full Professor of Physical Chemistry, Federico II University of Naples (1994-2008)
1994 Visiting Professor at Ecole Normale Superieure (Paris) and CEA-CENG (Grenoble)
1990 Associate Professor of Physical Chemistry, Federico II University of Naples (1982-1993)
1982 Post-Doc, University Erlangen-Nürnberg (Germany)
1981 Post-Doc, University of Montreal (Canada)
1980 Assistant Professor of General Chemistry, University of Calabria (1979-1981)
1979 Post-doc at CEA-CEN, Grenoble, France
1978 Post-doc at Erlangen-Nurnberg University, Germany
1977 *Degree in Chemistry, University Federico II of Naples*
1976 Military Service, Italian Air Force
Born in Ancona, Italy
1952

Apart from Italian (mother tongue) Barone is fluent in both English and French

Bibliometric Data

Barone has authored more than 750 papers in ISI journals and several book chapters with more than 50000 citations (4252, 4443, 4925, 4597 and 4585 in 2013, 2014, 2015, 2016, and 2017, respectively), an average citation per item of 73 and an h-factor of 82 (60 for papers published since 2000, 43 since 2005, and 28 since 2010); 10 papers were cited more than 1000 times and 68 papers more than 100 times each. The most significant scientific contributions include fundamental developments in Density Functional Theory, solvation theory, and computational spectroscopy, together with state-of-the-art applications in materials chemistry, life sciences, nanosciences and cultural heritage.
A full publication list is available at: http://dreams.sns.it
Here below are given some key information.

List of the top 10 publications in the last 10 years (in chronological order)

Publications	***Citations***
• V. Barone, *Anharmonic vibrational properties by a fully automated second-order perturbative approach*, J.Chem.Phys. **122**, 014108 (2005).	741
• G. Scalmani, M. J. Frisch, B. Mennucci, J. Tomasi, R. Cammi, V. Barone, *Geometries and properties of excited states in the gas phase and in solution: Theory and application of a time-dependent density functional theory polarizable continuum model*, J.Chem.Phys. **124**, 094107 (2006).	527
• R. Improta, V. Barone, G. Scalmani, M.J. Frisch, *A State-Specific PCM TD-DFT method for equilibrium and non equilibrium excited state calculations in solution*, J.Chem.Phys. **125**, 054103 (2006).	292
• F. Santoro, R. Improta, A. Lami, J. Bloino, V. Barone, *Effective method to compute Franck-Condon integrals for optical spectra of large molecules in solution*, J. Chem.Phys. **126**, 084509 (2007).	242
• T. Gustavsson, A. Banyasz, E. Lazzarotto, D. Markovitsi, G. Scalmani, M. J. Frisch, V. Barone, R. Improta, *Singlet excited-state behaviour of uracil and thymine in aqueous solution: A combined experimental and computational study of 11 uracil derivatives*, J.Am.Chem.Soc. **128**, 607-619 (2006).	240
• Barone, Vincenzo; Casarin, Maurizio; Forrer, Daniel; et al., *Role and Effective Treatment of Dispersive Forces in Materials: Polyethylene and Graphite Crystals as Test Cases*, Journal Of Computational Chemistry, **30**, 934-939 (2009)	230
• Improta, Roberto; Scalmani, Giovanni; Frisch, Michael J.; et al., *Toward effective and reliable fluorescence energies in solution by a new state specific polarizable continuum model time dependent density functional theory approach*, Journal Of Chemical Physics, **127**, 074504 (2007)	200
• F. Santoro, A. Lami, R. Improta, J. Bloino, V. Barone, *Effective method for the computation of optical spectra of large molecules at finite temperature including the Duschinsky and Herzberg-Teller effect. The Q_x band of porphyrin as a case study*, J.Chem.Phys. **128**, 224311 (2008).	185
• V. Barone, J. Bloino, M. Biczysko, F. Santoro, *Fully integrated approach to compute vibrationally resolved optical spectra: from small molecules to macro systems*, J.Chem.Theory Comput. **5**, 540-554 (2009).	181

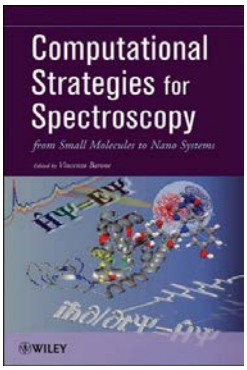
- F. Santoro, A. Lami, R. Improta, J. Bloino, V. Barone, *Effective method to compute vibrationally resolved optical spectra of large molecules at finite temperature in the gas phase and in solution*, J.Chem.Phys. **126**, 184102 (2007). 165

List of other 15 key publications (in chronological order)

Publication	***Citations***
• P. Corradini, V. Barone, R. Fusco, G. Guerra, *A Possible Model of Catalytic Sites for the Stereospecific Polymerization of α-olephins on First Generation and Supported Ziegler-Natta Catalysts*, Gazzetta Chimica Italiana **113**, 601-607 (1983).	94
• E. Benedetti, V. Toniolo, P. Hardy, V. Barone, A. Bavoso, B. Diblasio, P. Grimaldi, F. Lelj, V. Pavone, C. Pedone, *Folded and Extended Structures of Homooligopeptides from α,α-dialkylated Glycines: a Conformational Computation and X-ray Diffraction Study*, J.Am.Chem.Soc. **106**, 8146-8152 (1984).	113
• V. Barone, C. Adamo, F. Lelj *Conformational Behaviour of Gaseous Glycine by a Density Functional Approach*, J.Chem.Phys. **102**, 364-370 (1995).	169
• C. Adamo, V. Barone, *Exchange Functionals with Improved Long-range behaviour and Adiabatic Connection Methods without Adjustable Parameters: the mPW and mPW1PW Models*, J.Chem.Phys. **108**, 664-675 (1998).	2016
• V. Barone, M. Cossi, *Quantum Calculation of Molecular Energies and Energy Gradients in Solution by a Conductor Solvent Model*, J.Phys.Chem. A **102**, 1995-2001 (1998).	4252
• C. Adamo,V. Barone, *Toward Reliable Density Functionals Without Adjustable Parameters: the PBE0 Model*, J.Chem.Phys. **110**, 6158-6170 (1999).	5517
• M. Cossi,V. Barone, *Time-dependent Density Functional Theory for Molecules in Liquid Solution*, J.Chem.Phys. **115**, 4708-4717 (2001).	1133
• M. Cossi, G. Scalmani, N. Rega, V. Barone, *New developments in the Polarisable Continuum Model for quantum mechanical and classical calculations on molecules in solution*, J.Chem.Phys. **117**, 43-54 (2002).	1649
• M. Cossi, N. Rega, G. Scalmani, V. Barone, *Energies, Structures, and Electronic Properties of Molecules in Solution by the C-PCM Solvation Model*, J.Comp.Chem. **24**, 669-681 (2003).	3459
• R. Improta, V. Barone, *Interplay of Electronic, Environmental, and Vibrational Effects in Determining the Hyperfine Coupling Constants of Organic Free Radicals*, Chem.Rev. **104**, 1231-1253 (2004).	253
• M. Biczysko, G. Scalmani, J. Bloino, V. Barone, *Harmonic and anharmonic vibrational frequency calculations with the double-hybrid B2PLYP method. Analytic second derivatives and benchmark studies*, J.Chem.Theory Comput. **6**, 2115-2125 (2010).	115
• J. Bloino, M. Biczysko, V. Barone, *General perturbative approach for spectroscopy, thermodynamics and kinetics: methodological background and benchmark studies*, J.Chem.Theory Comput. **8**, 1015-1036 (2012)	85
• A. Baiardi, J. Bloino, V. Barone, *General Time Dependent Approach to Vibronic Spectroscopy Including Franck-Condon, Herzberg-Teller, and Dushinsky Effects*, J.Chem.Theory Comput. **9**, 4097-4115 (2013)	62
• V. Barone, M. Biczysko, J. Bloino, *Fully anharmonic IR and Raman spectra of medium-size molecular systems: accuracy and interpretation*, Phys.Chem.Chem.Phys. **16**, 1759-1787 (2014)	101

- D. Licari, A. Baiardi, M. Biczysko, F. Egidi, C. Latouche, V. Barone, *Implementation of a Graphical User Interface for the Virtual Multifrequency Spectrometer: the VMS-Draw Tool*, J.Comput.Chem. **36**, 321-334 (2015) 25

Five selected research monographs and chapters in collective volumes (last 5 years)



- A. Salvadori, D. Licari, G. Mancini, A. Brogni, N. De Mitri, V. Barone, Graphical Interfaces and Virtual Reality for Molecular Sciences, Reference Module in Chemistry, Molecular Sciences and Chemical Engineering, Elsevier 2014.
- V.Barone, M.Biczysko, I.Carnimeo, Computational Tools for Structure, Spectroscopy and Thermochemistry, in *Understanding Organometallic Reaction Mechanisms and Catalysis*, V.P. Ananikov, Ed., Wiley-VCH, 2015, pag.249-320.
- V. Barone, Ed. *Computational Strategies for Spectroscopy: from Small Molecules to Nanosystems*. John Wiley & Sons, 2012.
- V. Barone, M. Biczysko, P. Cimino. "Interplay of Stereo electronic Vibrational and Environmental Effects in Tuning Physicochemical Properties of Carbon-Centred Radicals". In *Carbon-Centred Free Radicals and Radical Cations*, M. D. E. Forbes, Ed., John Wiley & Sons, 2010, pp. 105-139
- V. Barone, M. Biczysko, G. Brancato. "Extending the Range of Computational Spectroscopy by QM/MM Approaches. Time-dependent and Time-independent routes". In *Combining Quantum Mechanics and Molecular Mechanics. Some Recent Progresses in QM/MM*, J. Sabin, S. Canuto, Eds., Advances in Quantum Chemistry Vol. 59. Academic Press, 2010, pp. 17-56

Five selected invited presentations (last 5 years)

- Virtual instruments for molecular sciences: the challenge of a multifrequency spectrometer, Yale University, December 10, 2015.
- Time dependent and time independent approaches to computational spectroscopy, CECAM Workshop, Paris, April 7-10, 2015.
- Toward a robust and user-friendly multifrequency virtual spectrometer, Genève, December 2012.
- Time dependent and time independent approaches to computational spectroscopy, 8th Seminar of Advanced Studies on Molecular Design and Bioinformatics (SEADIM 8). Cuba, July 2011.
- Calculation of magnetic tensors and EPR spectra for free radicals in different environments, SPIN2011, Marseille, June 2011.

Five selected memberships in committees of international conferences (last 5 years)

- Chair of the Meetings of COST Action CM1002: COnvergent Distributed Environment for Computational Spectroscopy (CODECS). Bratislava, 2014; Madrid 2013; Porto, 2012; Paris, 2011; Pisa, 2011.
- Member of the Organizing and Scientific Committee of the International Congress Energy from the Sun, Chia Laguna (2012).
- Chair of the Avogadro Colloquia: Bologna (2012), Pisa (2013).
- Chair of XXIII e XXIV Congresses of the Società Chimica Italiana, Sorrento (2009) e Lecce (2011).
- Chair of "Winter Modelling" workshops. Roma 2007; Pisa 2008, 2010, 2011, 2012, 2014, 2015.

Curriculum Vitae

Vincenzo Barone was born in Ancona, Italy on November 8, 1952. After graduating in chemistry (1976, summa cum laude), he continued his education at the Universities of Marseille, Grenoble, Paris, Erlangen-Nurnberg, Montreal and Berkeley. He became Associate Professor in 1982 and Full Professor in Physical Chemistry in 1994 at the Federico II University of Naples. Since 2008 he serves as Full Professor in Theoretical and Computational Chemistry at the Scuola Normale Superiore.

Scientific Activity

The main research interests of Barone 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 an integrated tool for the accurate description of physical-chemical processes in condensed phases - including a general and powerful electronic model (the result of the development of original and effective approaches in the framework of the density functional theory), an accurate description of solute-solvent interactions (through mixed discrete-continuum models), and the inclusion of the most important effects of nuclear motions (vibrational averaging of physical-chemical observables, reaction rates, vibronic structures, slow motions). Particular attention has been devoted to obtaining a computational accuracy comparable to the one attainable through experiments, without losing the possibility of an interpretation in terms of basic chemical-physical models and simple general rules. The focus on realistic systems has typically implied "multiscale" approaches, i.e. the adoption of several theoretical models suitable for different scales of a specific phenomenon, and their integration into more comprehensive descriptions. Such an approach has moreover triggered a constant interest in computer architectures and, in the last years, grid implementations. Such a research strategy, located at the crossway of theoretical and computational chemistry, has aimed at developing a number of integrated computational tools. Starting from accurate and cost-effective methods for electronic structure calculation, such tools take next into account both environmental effects through integrated discrete-continuum approaches, and nuclear motions through models ranging from classical Molecular Dynamics (MD) to both time-dependent (TD) and time-independent (TI) quantum dynamics. A strong feeling for the interpretation of experimental results is evidenced by long-standing collaborations with top-level experimental groups. A constant effort has been devoted to making theoretical developments available in form of general and easily accessible computational tools.

Areas in which Barone has provided remarkable contributions include:

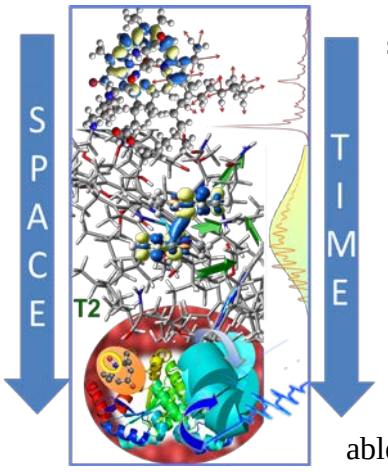
1) Density functional theory: (i) Development and validation of new density functionals (e.g. the mPW1PW and PBE0 hybrid functionals (*J. Chem. Phys.* 108, 664 (1998); *J. Chem. Phys.* **110**, 6158 (1999)); these have been employed in more than 500 scientific studies in the last 5 years; (ii) Validation of DFT for molecular spectroscopy studies; in particular, contributions concerning open shell molecules are widely recognized (*Chem. Rev.* **104**, 1231 (2004)); (iii) Implementation and parameterization of tight-binding (TB) DFT and of its time dependent (TD) extensions (TB-TD-DFT) allowing for a wider range of applications involving both ground and excited electronic states (*J. Chem. Theory Comput.* **7**, 713 (2011), and **7**, 3304 (2011)).

2) Solvation theory: Several contributions to the development of the Polarisable Continuum Model (PCM): (i) Improvement of the model for the calculation of solvation free energies (*Chem. Phys. Lett.* **255**, 327 (1996), *J. Phys. Chem. A* **102**, 1995 (1998)); (ii) Implementation of analytical derivatives allowing geometry optimizations in solution (*J. Comput. Chem.* **19**, 404 (1998)); (iii) Extension of the model to the description of excited electronic states (*J. Chem. Phys.* **115**, 4708 (2001); *J. Chem. Phys.* **124**, 094107 (2006)); (iv) Linear scaling implementation paving the way to the study of macromolecules in solution (*Theor. Chem. Acc.* **111**, 90 (2004)); (v) Development of mixed discrete-continuum models for

computational spectroscopy, by both time-independent and time-dependent approaches (General Liquid Optimized Boundary (GLOB) model, *Theor. Chem. Acc.* **117**, 1001 (2007) and integration of floating charges in the discrete layer, *J. Chem. Theory Comput.* **8**, 4270 (2012); *J.Comput.Chem.* **31**, 2271 (2015)). These advances and (vi) their implementation in popular computational packages have greatly contributed to make PCM the most widely used method for quantum mechanical studies of molecules in condensed phases.

3) Molecular vibrations: Effective treatments of harmonic and anharmonic contributions for processes involving single (vibrational terms, *J. Chem. Phys.* **101**, 10666 (1994); *J. Chem. Phys.* **120**, 3059 (2004); *J. Chem. Phys.* **122**, 014108 (2005); *J.Chem.Phys.* **136**, 124108 (2012); *J.Chem.Theory Comput*. **8**, 1015 (2012); *PCCP* **16**, 1759 (2014); *Int. J. Quantum Chem*. **115**, 948 (2015); *J.Phys.Chem. A* **119**, 11862 (2015)) as well as multiple (vibronic effects, *J. Chem. Phys.* **126**, 084609 (2007); *J.Chem.Theory Comput.* **9**, 4097 (2013); *J.Chem.Phys.* **141**, 114108 (2014); *J.Chem.Phys.* **143**, 204102 (2015); *J.Chem.Theory Comput.* **11**, 3267 (2015)) electronic states, implemented as independent plugins.

4) Computational spectroscopy: The research activity in this area builds on, and provides a unifying frame for, all the above-mentioned topics. Specific developments, paving the way to the reproduction of spectral line-shapes, concern the effect of large amplitude nuclear motions on spectroscopic observables, and the computation of vibrationally resolved electronic spectra (absorption, emission, circular dichroism, and resonance Raman) for large molecular systems in condensed phases (*Proc. Natl. Acad. Sci. USA* 104, 9931 (2007); *Angew. Chem.* **46**, 405 (2007); *Acc. Chem. Res.* **41**, 605 (2008); *J.Phys.Chem.Lett.* **3**, 1766 (2012); *J.Chem.Theory Comput.* **9**, 1880 (2013); *Inorg.Chem.* **54**, 5588 (2015)). In the field of ESR spectroscopy, development of a number of computational tools (*Theor. Chim. Acta* **91**, 113 (1994); *J. Chem. Theory Comput.* **4**, 751 (2008); *Mol.Phys*. **111**, 1345 (2013)) has allowed to account for all the chemical/physical effects modulating the spectral observables, and to compute entire spectra (as opposed to individual parameters) in agreement with experiments (*Phys. Chem. Chem. Phys.* **8**, 4609 (2006); *J.Am.Chem.Soc.* **129**, 11248 (2007); *J.Chem.Theory Comput*. 9, 3626 (2013)).



This methodological machinery has been employed to describe many systems and processes coupling accuracy comparable to that of the reference experiments with interpretability of the results in terms of molecular models and general rules. The focus has been on relatively fast “local” phenomena tuned by long-range intra- and inter-molecular interactions with comparable or longer characteristic time scales. Space and time multi-scale approaches are particularly well adapted to these problems and have been at the heart of the research philosophy of Barone, leading to integrated global descriptions of increasing sophistication and reliability, with the perspective of building and validating a new generation of virtual instruments for molecular sciences with unprecedented effectiveness. In this connection, the virtual multi-frequency spectrometer (VMS) is already able to deal with several widely used spectroscopies (nuclear and electron magnetic resonances, microwave, vibrational and electronic, the last two including also chiral techniques) and is completed by the powerful VMS-Draw graphical user interface (*Chemphyschem* **15**, *3355 (2014); Chirality* **26**, 228 (2014); *J.Comp.Chem*. **36**, 321 (2015); *J.Chem.Theory Comput.* **11**, 4342 (2015), (2015)). Barone has always advocated the necessity of making innovative theoretical and computational methods available well beyond the circle of developers, especially towards the community of experimental researchers, that often have at hand highly interesting, challenging applications, which require appropriate computational/theoretical assistance.

In the last two years the new research topic of astrochemistry and molecular astrophysics has become increasingly significant with special reference to the simulation of kinetic and spectroscopic features of prebiotic molecules. This activity has led to a number of papers in specialized journals (e.g. *Astrophys.J.* **785**,107 (2014); **792**,118 (2014); **810**,111 (2015)) and also to a first review (*Acc.Chem.Res.* **48**, 1413 (2015)).

The scientific activity of Vincenzo Barone and his group, and his research leadership in the field of theoretical/computational chemistry is evidenced by the large number of contributions to the most influential scientific journals in chemistry (*Chem. Rev., Accounts Chem. Res., Proc. Natl. Acad. Sci. USA, Chem. Soc. Rev., Angew. Chem. Int. Edit., J. Am. Chem. Soc., Chem-Eur. J.*), with special reference to

chemical physics and theoretical chemistry (*J. Phys. Chem., J. Chem. Phys., J. Comput. Chem., Chem. Phys. Lett., ChemPhysChem., Phys. Chem. Chem. Phys., J. Chem. Theory Comput.*). Barone has authored more than 700 publications in international journals, and during the last 10 years has given more than 80 invited lectures at Italian and foreign institutions (with a total of more than 150 during his whole career). His publications have received more than 43000 citations (3496, 3943, 4248, 4469 and 4583 in 2011, 2012, 2013, 2014, and 2015, respectively), an average citation per item of 61.5 and an h-factor of 76 (60 for papers published since 2000, 43 since 2005, and 28 since 2010); 8 papers were cited more than 1000 times and 57 papers more than 100 times each. Both the number of citations and the h-index has been hugely increasing in the last years.

In 2009 Barone was included among the ISI *highly cited* researchers for the Chemistry category. In the same year he has obtained the *Luigi Sacconi* medal, which is awarded to chemistry scientists of international fame. In 2008 he was elected as member of the International Academy of Quantum Molecular Science, whose members are chosen among the scientists of all countries who have distinguished themselves by the value of their scientific work, their role of pioneers or leaders of a school, in the broad field of the application of quantum mechanics to the study of molecules and macromolecules. In 2013 Barone was elected as fellow of the Accademia dei Lincei, whose members are chosen among the top Italian scientists of different fields. The research activity of Barone has attracted numerous grants from commercial and academic institutions, the Italian Ministry of Education, University and Research and the EU. He is *Fellow* of the *Royal Society of Chemistry*, member of the *American Chemical Society* and of the *American Institute of Physics*, associated member of the Physical Chemistry and Biophysics Division (I) of IUPAC, member of the Scientific Boards of IRSAMC (*Institut de Recherche sur les Systèmes Atomiques et Moléculaires Complexes*, Toulouse, France), of the Chemistry Department of CNRS (France), and of the Doctoral School of the Padua University.

Management Experiences

From 2013 until 2016 (when he has been appointed as Director of the Scuola Normale Superiore) Barone directs one of the leading research groups in the field of theoretical/computational Chemistry. The group is structured in the DREAMS (Dedicated Research Environment for Advanced Modelling and Simulations) support centre of the Scuola Normale Superiore (http://dreams.sns.it) and it includes Researchers coming from the Scuola Normale Superiore itself as well as from the CNR (National Research Council) and from the INSTM consortium. One of the main activities of the DREAMS centre concerns high-resolution 3D technology and a Cave Automatic Virtual Environment, which make possible the interactive manipulation of virtual "objects" on scales ranging from the cosmological down to the molecular size. The approaches of virtual reality are also a fertile ground for reconciliation between the hard sciences and the humanities, both traditional areas of excellence within the Scuola Normale Superiore. Examples of such collaboration include applications aimed at the reconstruction of archaeological contexts, the integration of the results obtained by different diagnostic techniques on works of art, virtual restoration, virtual reconstruction of the processes underlying the creation of images and works of art, etc.

It should be stressed here that, since his appointment at the Scuola Normale Superiore in 2009, Barone has devoted an intense and successful effort to root chemical disciplines in the scientific and educational offer of this prestigious institution. In particular, the research group directed by Barone has rapidly achieved a remarkable size in terms of personnel; the group has moved in 2012 to the premises of the renovated headquarters of Palazzo D'Ancona, where dedicated spaces and equipment (offices, classrooms and computer rooms) have been established and organized. The increased role of chemistry and the recognition of the activity of Barone are witnessed also by his election in 2015 as Dean of the Classe di Scienze Matematiche e Naturali and, in 2016, as Director of the Scuola Normale Superiore.

The direction of the DREAMS centre allows Barone to manage delocalized computational resources on a city-wide scale; on a national scale he coordinates the Virtual Integrated Laboratory for Large-Scale Applications in a Geographically-distributed Environment (M3-VILLAGE; http://m3village.sns.it), with nodes in several University Departments as well as in Institutes of the Italian National Research Council. Finally, at an international level, he directs the SNS node of the European Centre for Atomic and

Molecular Computations (CECAM, www.cecam.org). The creation of such virtual laboratories is inspired by the grid- and cloud-computing paradigms, not only in terms of sharing and merging of local computational resources, but also, at a more fundamental level, in the creation of a network of researchers with diverse complementary experience, ranging from quantum mechanical methods to statistical/stochastic approaches and analytical techniques. All these "tools" are organized under Barone's coordination, in order to create truly multi-scale approaches capable of providing reliable computational descriptions of challenging, real-life systems and processes. Barone is also member of the Management Board of the Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali (INSTM).

Barone has been the principal proponent and the Chair of the Management Committee of the COST Action CM1002: COnvergent Distributed Environment for Computational Spectroscopy (CODECS, www.idea.sns.it/CODECS), an interdisciplinary Project financed under the Chemistry and Molecular Sciences and Technology COST Domain, that extends over the 2010-2014 period, and featured 21 signatory countries, for a total of over 50 international research institutions. The main aim of CODECS was to promote scientific interchange / interconnection within the community of European researchers working in the area of computational spectroscopy, and to organize their activities into a network.

Barone has been the coordinator of the Chemistry Ph.D. program at the Scuola Normale Superiore since 2009. In 2014 this program has been completely reshaped and focussed on the development, and validation of new theoretical and computational methods and to their application in several fields, including astrochemistry, cultural heritage, nanosciences and life-sciences. This change is witnessed by the new name (Methods and Models for Molecular Sciences) and by the involvement in the program of several leading researchers from Italy and abroad. Barone has supervised more than 35 Ph.D. students and over 25 post-doc researchers; many of them, including -notably- several female scientists, have brilliantly proceeded in their scientific career. Among those who work in academic environments, we cite Carlo Adamo (Full Professor, EN-SCP, Paris), Maurizio Cossi (Associate Professor, University of Eastern Piedmont), Roberto Improta (Senior Research Scientist, CNR), Nadia Rega (Associate Professor, Federico II University of Naples), Paola Cimino (Researcher, University of Salerno), Julien Bloino (Research Scientist, CNR). Other past-members of the group carry out research activities within private companies, e.g. Dr. Giovanni Scalmani (now at Gaussian, Inc.).

Barone's research activity has always attracted grants from public and private institutions, including, in recent years:

- Ideas ERC Advanced Grand DREAMS (2013-2017; 2200000 euros);
- Hi-Life PON Project (2012-2015, overall budget for SNS activities ca. 800000 euros)
- CECAM [2011-2014 (200000 euros allocated to the SNS node) and 2015-2018 (320000 euros allocated to the new SMART node leaded by SNS)];
- SNS Grant [2011-2012 (85000 euros), 2013-2014 (55000 euros) and 2015-2016 (55000 euros)];
- COPAC project of the Tuscany Region (2011-2013; 450000 euros for the SNS unit);
- POLOPTEL CARIPI project (2011-2013; 80000 euros allocated to the SNS unit);
- Research agreement with Gaussian, Inc., USA (budget 36000 $/year).

Many projects involve explicit consequences in terms of technology transfer of research results. Examples where such links are particularly noticeable are the COPAC project aimed at restoration of contemporary artworks and creation of a dedicated database, funded by the Tuscany Region for 2011-2013; the POLOPTEL project, devoted to the design of new polymer systems to produce materials and devices for smart applications, funded by Fondazione Cassa di Risparmio di Pisa for the 2011-2013 period; PODIME, a project for the development of memory devices based on polymers, funded in 2006 under "Law 297", with ST Microelectronics and the IMAST technological district of the Campania Region; and the SCoPE project, aimed at creating an infrastructure for distributed high performance computing for scientific and technological applications, funded under PON 1575/2004.

A remarkable ability in designing and implementing large and inclusive platforms, capable of stimulating and organizing the sharing of ideas, resources and results among researchers active at the frontier of computational modelling, is witnessed inter alia by numerous initiatives at the national and international level.

In this perspective, we mention the direction of a Node of CECAM (*Centre Européen de Calcul Atomique et Moléculaire*) at the Scuola Normale Superiore, inaugurated in 2011; the chairmanship of the COST Action "Convergent Distributed Environment for Computational Spectroscopy" (CODECS), aimed

at creating an international network of research groups active in the field of computational spectroscopy, with the current participation of more than twenty European countries, and the organization of the "Winter Modelling" series of Meetings, which on a yearly basis gather at the Scuola Normale Superiore researchers working in the field of bottom-up modelling of complex molecular systems.

The management activities conducted at the national and international level for the promotion of chemistry, not only in its relationships with other scientific and technological fields, but also with respect to the cultural and social perception, is demonstrated by several positions held in the Italian Chemical Society: he was Coordinator of the Interdivisional Group on Computational Chemistry (2004-2006), Chairman of the Division of Chemical Physics (2007-2009), and is currently President of the Italian Chemical Society for the 2011-2013 period. In this capacity, he has coordinated several initiatives related to the celebration of the International Year of Chemistry (IYC 2011): even the scientific inauguration of the International in Italy was held at the Scuola Normale Superiore in February 2011.

Some of these initiatives are aimed at a broad audience, going beyond traditional disciplinary and cultural boundaries: thus, the lecture series "Chemistry is … Chemistry and...", hosted by the Scuola Normale Superiore, explores from unusual viewpoints the links between chemistry and disciplines close to or (apparently) distant from it, such as Physics, Medicine, Biology, but also the Arts, Mathematics and Literature. Constructive interactions with many areas of research, technology transfer and industrial applications are also demonstrated by a dense series of public events. Although external actions to enhance the public image of chemistry are very important, they do not represent the essence of the program for the three-year presidency of the Italian Chemical Society (SCI). The most significant aspect is identified instead in the concrete revival of the scientific value of SCI, with a series of initiatives to foster the development of high-level research, and to bring out the results. The effort to recover the role of SCI as an interface between research, industry and social issues, culminated in the promotion of Networks aimed at creating a more systematic and more structured interaction among stakeholders and direct beneficiaries of the research in Italy - Academia, Research Institutes, Industrial Laboratories, Companies.

In 2008 Barone was Director of the Institute for Physical-Chemical Processes (IPCF), which is one of the largest CNR Institutes, with a staff of one hundred employees including more than 50 researchers with a background mainly in physics and chemistry. This strong interdisciplinary character, which represents a key feature of IPCF and is absolutely consistent with Barone's scientific vision, has been enhanced and emphasized under his directorship. The direction of IPCF, as well the coordination of Project 7 (see below), have allowed Barone to acquire a thorough understanding of staff management issues, also in relation to specific aspects of CNR.

In the period 2007-2010 he was Coordinator of the Project 7 of the Department of Molecular Design of CNR. Beyond even the relevant objectives of individual contracts, from a strategic point of view the project was conceived as an attempt to streamline the activities of computational modelling performed within DPM, in a non-sectorial perspective open to constructive interactions with external Institution (Universities, Consortia, Computing Centres, Companies, etc.) that express important computational modelling initiatives. The basic belief is that integration among these initiatives, partially overlapping, but complementary to a greater extent, can create virtuous synergies in Italy.

In 2013 he became Director of the new DREAMS centre at the Scuola Normale Superiore, which includes more than 30 researchers and technicians and is organized in two sections, dedicated to high-performance computing (HPC) and advanced virtual reality techniques (3D), respectively. In 2015 the HPC facilities have moved to the new Avogadro data centre, which represents the reference platform to run processor-intensive numerical simulations with large data sets, requiring parallel efficiency, scalability and fast memory access. This integrated computational facility includes about 5000 cores monitored in real time and linked to a huge amount of last generation data storage. These resources represent also the background of the virtual reality facilities, which offer to researchers and students most of the cutting-edge technologies in terms of 3D visualization, motion tracking and interactive environments (virtual and augmented reality).

Evaluation Activity

Barone has extensive experience in the evaluation of research projects, both national and international. He has been a member of Ph.D. committees in many European countries. In 2009 he was a member of the Board of Trustees for the evaluation of the PRIN projects of the Italian MIUR. He was the only Italian member of the Evaluation Committee of the University of Turin research projects in 2011.

He worked as a scientific project evaluator for the national funding agencies of the U.S. (National Science Foundation, NSF), Austria (*Fonds zur Förderung der wissenschaftlichen Forschung*, FWF), France (*Agence Nationale de la Recherche*, ANR) and Belgium (*Fonds de la Recherche Scientifique*, FNRS). As a member of the respective Scientific Advisory Boards, he participates in self-assessment activities of the Chemistry Department of CNRS (France) and of the Graduate School of Padua.

He is member of the Advisory Boards of *Spectrochimica Acta A, Theoretical Chemistry Accounts*, *Journal of Computational Chemistry*, and *Physical Chemistry Chemical Physics*: participation in these editorial boards involves inter alia the settling of disputed assessments concerning scientific contributions submitted to journals.

Barone has participated in several committees for comparative evaluations for the allocation of permanent positions in the Italian University in the sector of Physical Chemistry (CHIM/02). In 2010 he was Chairman of the Board of Senior Researcher CNR Selection for the “Chemistry” area. In all these procedures for recruitment, he has strongly supported the establishment of criteria based on internationally recognized indices (impact factor, h-index), a practice that over time has achieved widespread support from the scientific community, and that is also reflected in the recent legislation.

In the period 2012-2014 Barone has been the President of the Chemistry Panel of the National Agency for Research Evaluation (ANVUR). The recently established Agency is in charge of implementing and carrying out the process of evaluation of the Italian Universities and research Institutions, including the preliminary elaboration of general criteria.

Only Connect: Science and Innovation as keys of a sustainable future

Complexity is recognized as the mark of our times, which characterizes the type of problems we are faced with in a vast variety of domains and disciplines, such as scientific research in every field, social, political and economic organization, education, global/local cultural interactions, technological innovation, sustainable development. A second and connected mark of our times is high speed change that, together with complexity, raises a particularly urgent need to govern and strategically plan the future, especially in terms of the role a country wants to have in a number of definite fields.

One crucial issue affecting a great number of applied sciences in Italy, is the need of more efficiently and consistently structured interactions among all of the actors and stakeholders operating in a given field – e.g. Academia, public research Institutions, Industrial Laboratories, Companies. In the past, applied sciences - in Italy- have successfully addressed a huge range of individual challenges and specific urgent needs, especially in fields such as pharmacology, agriculture, manufacturing, energy, etc. Looking from a distance in time, this phase can be defined as "reactive" rather than proactive, and it has brought as a consequence that insufficient attention has been paid to issues such as the environmental impact and the medium and long-term sustainability of the production processes. These considerations have been gaining increasing importance in today’s perception, and the relationship between scientific research, technological innovation and sustainability is becoming a central aspect in any far-sighted development strategy. A full deployment of the potentialities of this new vision requires significant political energies and investments. The conversion of industrial processes to new modes of production must be governed and supported. Even more importantly, a close and robust model of interaction between industry, applied and curiosity-driven frontier research must be devised, decidedly sustained and fostered. The advantages of such a strategy are well demonstrated by what happened in a number of relevant cases, such as, for instance, the remarkable diffusion of biodegradable polymers, green building strategies, and environmentally friendly tanning processes. Such cases, however, are still limited in number and quite local in character.

Small and medium-size companies could benefit enormously from the possibility of interacting with high-level research capabilities, especially in regard to issues such as process and product innovation, competitiveness in the market, as well as sustainability and environmental impact. This holds especially

true if such an interaction is implemented not only on a short-term basis aimed at the solution of specific problems, but is instead turned into a medium- and long term- collaborative strategy, aimed at producing frontier research in the underlying scientific topics. Although such a strategy is the mandatory and crucial prerequisite to secure robust and sustainable industrial innovation on the long run, it remains typically beyond the reach of small and medium-size companies. A possible solution can be based on the creation of networks, a model of interaction that has been experimented with remarkable success mainly in fields different from industry.

Even research institutions would enormously benefit from a strategy based on networks. At present, research groups in the Academia and in public research Institutions are typically small and isolated, both in terms of human and instrumental resources. This circumstance often produces a situation of duplication and fragmentation. Formal, concrete and institutionalized collaborative networks can therefore be extremely advantageous in view of an efficient integration, rationalization and sharing of scientific knowledge, technological know-how, instrumentation and administrative skills (such as project management). Such a strategy can be instrumental in accessing funds (e.g. one granted on the basis of competitive calls), optimizing financial and human resources, existing structures and instrumentation. Finally, a network structure would allow putting technology-oriented funding programs, which are typically offered on a regional basis, within broader scientific contexts.

A necessary step of such a strategy would imply that a number of key sectors are identified primarily on the basis of prospective applications and foreseeable developments, but also possible strongly rooted local contexts. If adopted on a systematic scale, however, such a strategy would also produce some adverse effects, such as the risk to cause the impoverishment of a cultural and industrial landscape, which is at present extremely rich and diverse in terms of scientific research as well as technological applications. The paramount importance of a small number of selected fields (e.g. medicine, high energy physics, etc.) possibly justifies today's tendency to concentrate massive investments on them. On the other hand, a careful and long-sighted political vision should guide such a selection as to entail that investments focus on a well-devised and sufficiently ample spectrum of scientific and technological sectors, which are considered as necessary for the development of the Country. A carefully planned synergy of investments is required in order to foster scientific and technological contributions from a higher number of scientific areas and cultures: chemical sciences, cultural heritage disciplines or agribusiness disciplines could be representative examples of such a widened strategy of selection.

This line of reasoning can be followed down to the level of a single research field. Just to make an example, chemical sciences cover a vast scientific territory including synthesis and characterization of molecules, supramolecules, macromolecules and multiphase systems, processing technology and functional behaviour; study and application of nanosystems. These areas deserve ample support and appropriate investments both as specific individual domains and in the context of a multidisciplinary integrated framework. As a complement to this strategy centred on collaboration among disciplines, it is also useful to identify a small number of key sectors that should be covered in a more focused perspective, i.e. relying on scientific and management resources that are almost entirely rooted within a single discipline. Examples in this direction are sustainable processes and green chemistry, as well as the bottom-up approach to smart and composite materials. Even in these sectors, which are decidedly rooted within Chemical Sciences, complementary contributions from other disciplines and collaboration with internal and external partners should be possible and welcome.

Already mature sectors must of course be adequately backed. Far-sighted and proactive scientific policies, however, must also foster and support promising developing sectors, as identified on the basis of credible indicators. Computational modelling approaches and *in silico* design methods, for example, definitely qualify as such: they are fast, environmentally safe, inexpensive, and they are becoming increasingly reliable and widely adopted in research. There is little doubt that they will rapidly come to play a crucial role in the development of technological applications as well.

Apart from the fields selected as relevant through both reactive and proactive policies, the need should be stressed to safeguard reasonable space and conditions for curiosity-driven research, not only as a training ground for brilliant and creative minds, but also in a more practical sense, as a high-risk/ high-gain investment towards future, not-yet-foreseeable developments. In a number of past and recent cases, research efforts that started out without forecasting any practical application, have resulted into unexpected findings and applications of the utmost scientific, technological, socio-economic and cultural

relevance. Going back to the example of computational modelling, high-level results can only be obtained if a good balance is reached in terms of efforts and investments, between applications to specific systems and processes on the one side, and theoretical and algorithmic (curiosity - driven research), on the other side. To summarize, investing in research is a win-win strategy insofar as it can draw the horizon that allows us to keep moving towards our future while remaining competitive.