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A tribute to Vincenzo Barone



It is with great pleasure that we present this tribute for the Festschrift celebrating the accomplishments (so far!) of Professor Vincenzo Barone of the Scuola Normale Superiore (SNS), Pisa. To friends and collaborators, he is simply Enzo, and we will speak of Enzo here.

Enzo's autobiography in this issue outlines his education and scientific accomplishments as well as a personal narrative of his path to science. Chance certainly played a central role in this path, but creativity, enthusiasm, scientific intuition and determination have done the rest. According to Enzo's autobiography, chance led him to chemistry (instead of physics), chance led him to theoretical chemistry, and chance led him to start what is probably his most active and productive research line: computational spectroscopy. He started with electronic paramagnetic resonance (EPR) spectroscopy and

extended his interests to almost all spectroscopic techniques, always fascinated by the power of spectroscopy to thoroughly characterize – in a non-invasive way – a wide variety of molecular (and supramolecular) systems and processes. His career has been characterized not only by a fierce determination to broaden the range of spectroscopies that he is able to master, but also by efforts to make this expertise available to a large and vibrant community of scientists. In this direction, in the last decade, Enzo embarked upon the so-called VMS (Virtual Multifrequency Spectrometer) project, whose major goal is to transition computational spectroscopy from a strongly specialized research area to a general tool open to non-specialists. The involvement of Enzo in so many different aspects of computational spectroscopy is well reflected in many contributions of the Festschrift, these ranging from the simulation of linear, resonant and/or chiroptical spectra in broad energy regimes (from the microwave to X-ray, from rotational to electronic spectroscopy, passing through different facets of vibrational spectroscopy) to the support to experimental studies, and to a theme dear to Enzo, that of the interplay of experiment and theory.

Enzo served as professor at the University of Naples from 1982 to 2008 (associate 1982-1994, full 1995-2008). Those years witnessed important and widely acknowledged results, demonstrating that it was possible to be competitive at an international level despite having limited resources and working in the south of Italy. It was in the 1990s that he became interested in new models for extending methods of quantum chemistry from isolated molecules to condensed phase environments. This research direction led to his most cited studies: those dedicated to solute-solvent interactions based on the polarizable continuum model developed in Pisa by Jacopo Tomasi, whom Enzo considered as a mentor. Among the contributions to this special issue, several of them deal with molecular systems in complex environments which are treated by continuum, mixed explicit-implicit or periodic crystal approaches.

His tenure at the University of Naples was an extraordinarily productive period for Enzo. Another focus of his research was density-functional theory, which revolutionized the traditional approach to computational chemistry by enabling accurate studies of large-sized molecules. It was at the end of the 1990s when he published his most cited paper (more than 11500 citations), which concerns the PBE0 model: a parameter free density functional model. The relevance of DFT models is witnessed by the fact that DFT is applied in almost all studies gathered in this special issue, with the systems considered (either stable or reactive, either in the ground or excited state) ranging from

small molecules of atmospheric or astrochemical relevance, to molecular complexes, to large organic molecules or biomolecules, and to metal clusters and metalorganic species. This great diversity in the type of systems considered and studies performed well reflects the kaleidoscopic research interests of Enzo.

2008 marked a turning point in Enzo's career. He chose to leave Naples to lead a National Research Council (CNR) institute in Pisa. However a call to hire the first professor ever in chemistry at the Scuola Normale Superiore (SNS) came in the same year, and Enzo applied for and got that position. Thirty-plus years after failing the admission to the SNS as a chemistry student, Enzo somewhat ironically joined it as full professor in chemistry. Another beginning, another challenge. Starting from scratch, from a small office and no collaborators, Enzo's enthusiasm, scientific intuition and determination led him to establish important new research lines, a large research group and a new laboratory (DreamsLab center which subsequently became the SMART Laboratory). The new themes concerned cultural heritage and the origin of life in the Universe, and he decided to tackle these challenges with an innovative approach: the integration of theory, experimentation, simulation, data science and virtual reality.

As those closest to Enzo know, he is still (and will always be) ready for new challenges. Enzo is now trying to extend his vision to the newly established Scuola Superiore Meridionale (SSM) in Naples. We have come full cycle: SNS and SSM involved together in projects and doctoral schools, the two cities of Enzo's academic and scientific career are now connected.

Besides being an outstanding scientist, Enzo cares for our community at large and has taken on roles of responsibility over his entire career. Over the course of the years he has trained several generations of Italian theoretical chemists who are now successful scientists in Italy and all over the world. Enzo has been very influential in their careers in the sense that he has taught them the importance of both developing state-of-the-art theories and working on challenging applications, and always going outside their comfort zone in research and being innovative.

This issue (the Vincenzo Barone Festschrift) contains over 60 manuscripts dedicated to our dear friend Enzo. They have been submitted by colleagues, former students and postdocs. We think they offer a clear idea of the impact that Enzo has had on different fields. Manuscripts submitted indeed range from method developments in quantum chemistry to structural and benchmark studies, to spectroscopic investigations (either computational or integrated with experiment) of isolated species or systems in condensed phases.

In closing, we congratulate Enzo for his inspiring and phenomenal academic accomplishments and wish him a joyful and healthy future!

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