Preface to the special collection in honour of Vincenzo Barone

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Published online: 5 June 2012
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The 60th birthday of Vincenzo Barone

Vincenzo Barone is Full Professor in Theoretical and Computational Chemistry at the Scuola Normale Superiore of Pisa and President of the Italian Chemical Society (SCI). Vincenzo Barone was born in Ancona (Italy) on November 1952. After his high school education, Enzo (as his friends call him) studied at the Department of Chemistry of the University of Naples, and in 1976, he received his degree (Laurea) in Chemistry discussing the thesis under the supervision of Professor Giuseppe Del Re, one of the pioneers of theoretical chemistry in Italy. He then moved as post-doctoral fellow to the University of Grenoble (France) where he worked under the supervision of Professor Robert Subra. We can date back to this period his interest in the chemistry of organic radicals, a field in which over the years he has produced major and widely recognized contributions.

From 1978 to 1981, Enzo was Assistant Professor in General Chemistry at University of Calabria (Italy), where he contributed to the creation of the Laboratory of Theoretical and Computational Chemistry (currently led by Professor Nino Russo). During this time, he was visiting scientist in well-known international Laboratories in France (Ecole Normale Supérieure, Paris; Université Joseph Fourier, Grenoble), Canada (Université de Montreal) and Germany (University of Erlangen-Nürnberg).

After a period as Associated Professor at the University of Naples, he become Full Professor of Theoretical Chemistry in 1994. In Naples, Enzo created the Theoretical and Computational chemistry group in which many young researchers found a fertile substrate for learning and working in exciting research fields. In few years, the group reached a remarkable reputation in the international
Scientific initiatives (e.g. the M3-Village Networks, the Idea
around the world. Scientists in universities and research centres in Italy and
and post-doc fellows are now professors and/or leading
with enthusiasm and efficacy. Many of his former students
ensured a congenial atmosphere, allowing the team to work
from all over the world. To all the co-workers, Enzo always
guest scientists, graduates, post-graduates and post-docs
universities in Italy.

In the last years, Enzo has promoted a number of sci-
initiatives (e.g. the M3-Village Networks, the Idea
Virtual Laboratory and the CODECS COST Action) that
have strongly contributed to the development of theoretical
and computational chemistry in Italy and in Europe. Fur-
thermore, he has played a seminal role in the creation of the
Computational Chemistry Division of the Italian Chemical
Society.

His scientific profile is really impressive: he is author of
more than 500 papers, which have received over 25,000
citations, with an h-index of 64; in 2009, he was included
among the ISI highly cited researchers for the Chemistry
category.

Enzo was also invited to hundreds of lectures in national
and foreign institutions or congresses, and he is member of
the editorial board of prestigious journals (e.g. Phys. Chem.
scientific council of many scientific institutions, fellow of
the International Academy of Quantum Molecular Science
and of the Royal Society of Chemistry, and chairman of
different national and international scientific events. Fur-
thermore, he is a co-author of Gaussian, one of the most
popular quantum chemistry codes.

Recently, he has received the prestigious Sacconi Medal
of the Italian Chemical Society for his contribution to the
development of theoretical and computational chemistry.

Of equal importance is the educational activity of Enzo:
until now, he has been supervisor of about 20 master and
more than 15 PhD students and has directed over 20 post-
docs in modern theoretical chemistry research.

Enzo has developed his research activities in many fields
of theoretical and computational chemistry, with the
overall goal to establish a theoretical microscopic approach
for the study of structural, dynamic, spectroscopic and
reactive properties of materials, biomolecules and more in
general soft matter in complex environments. His contribu-
tions to the accurate description of solvent effects and
nuclear motions represent a logical element of this strategy.

Of particular interest is Enzo’s conception of theoretical
and computational chemistry as an “experimental” tool
that can be used not only to achieve chemical accuracy in
computed physico-chemical properties, but also to unravel
and understand phenomena at the atomistic level. This has
led Enzo to adopt in his research a strongly multidisci-
plinary approach, which is focused in the first place on
theoretical developments and on multiscale descriptions,
but also addresses the potentialities of computer architec-
tures and grid implementations.

More in details, the areas in which Enzo has provided
remarkable contributions include the following:

- Chemical bond and molecular reactivity. In this con-
text, we only mention the work on the absorption of
atoms and molecules on solid surfaces, the chemical
properties and reactivity of radical species, conforma-
tional analysis and photo-electron spectroscopy of
biphenyl-like systems;

- Density functional theory (DFT). Already in 1992,
Enzo was convinced of the potential of density
functional theory to deal with chemical problems. His
contributions include the development and validation of
new exchange–correlation functionals (such as
mPW1PW and PBE0), the validation of DFT for
open-shell systems and, more recently, the imple-
mentation and parameterization of tight-binding DFT and
of its time-dependent extension;

- Solvation theory with special emphasis on the polariz-
able continuum model (PCM). The approach has been
developed and implemented for the evaluation of
solvation free energies, including solvent effects on
molecular structures in both ground and excited elec-
tronic states. In the last years, he has also been involved
in the development of a mixed discrete-continuum
model especially useful for computational spectroscopy
applications. Enzo’s work in this field has contributed
to make of PCM the most widely used tool to study
cellular systems in condensed phases at quantum
mechanical level;

- Computational spectroscopy. Enzo’s studies on har-
monic and anharmonic treatments of molecular vibra-
tions paved the route to unprecedented results in the
field. In the last years, his scientific interests have
focused on theoretical developments instrumental to the
accurate simulation of spectral line-shapes for large
molecular systems in condensed phases; as an example
of the potential of the approach, one can cite the
computation of entire EPR spectra of different molec-
ular systems, in excellent agreement with the exper-
imental counterparts.

This short extract of the Enzo’s scientific contributions
is inevitably reductive; the interested reader will easily find
in the current literature his fundamental contributions to the advancement of Theoretical and Computational Chemistry. We are therefore confident that in the next decades, Enzo Barone will continue to develop and apply new theoretical approaches and will thus keep contributing to a better knowledge of Chemistry.

Finally, we would like to underline the genuine personal character of Enzo, his ability to be a friend for his students, co-workers and colleagues, his helpful attitude and his broad cultural interests. For a long time, Enzo was a teetotaller, but over the last 20 years, he has become able to appreciate a glass of good wine. For this reason, we will accompany our wishes for his 60th birthday by opening a bottle of the best Italian wine in order to toast with all the numerous friends he has in the world. **Forza Enzo, sono solo i primi sessant'anni!** (Go Enzo, these are just the first 60 years!)

We are grateful to the many authors who contributed to this special issue of TCA dedicated to the 60th birthday of Enzo Barone and to the numerous referees who have dedicated their valuable time to evaluate the manuscripts. We are also grateful to Christopher Cramer for his enthusiastic acceptance of our proposal for this special issue and to the TCA staff for its help all along the editorial work.
Vincenzo Barone
A Festschrift from Theoretical Chemistry Accounts
Russo, N.; Rega, N.; Adamo, C. (Eds.)
2013, VII, 359 p. 225 illus., 113 illus. in color.,
Hardcover
ISBN: 978-3-642-34461-9