A EUROPEAN JOURNAL

CHEMPHYSCHEM

OF CHEMICAL PHYSICS AND PHYSICAL CHEMISTRY

17/2011

EDITORIAL

DOI: 10.1002/cphc.201100862

Recent Progress in Theoretical and Computational Chemistry

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Theoretical and Computational Chemistry has seen a remarkable development in the past decades. While it started as a discipline of a few experts in the 1960s, the field has grown enormously due to advances in computational resources and software packages. In addition to the dramatic increase in computer power, a wide range of methods with predictive capabilities such as density functional theory (DFT) turned out to be extremely valuable tools in the hands of those who understand the chemistry of the systems under study and the limitations of the methods. As a result, increasingly larger molecular systems are nowadays routinely studied and interpreted according to the fundamental principles of quantum mechanics, including studies of electronic structure and reactivity of complex molecular processes. At the same time, the development

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of new methods and density functionals continues to be a vibrant field of research in a sustained effort to develop reliable approaches for almost any problem in chemistry.

The availability of user-friendly software packages has popularized the field well beyond the realm of theoretical and computational chemistry groups. Today, almost any experimental research group in the world has an active member, or close collaborator, involved in computational modeling. The software packages are so popular and easy to use that calculations can be performed even by researchers with very limited knowledge of the underlying theories or approximations involved in the computations. While the calculations are easy to run, the interpretation of the resulting data, the range of validity of the approximations involved, and the range of error of the calculations performed with these popular software packages are often difficult to assess even by experienced users. These difficulties are exacerbated by the rapid emergence of new methods, acronyms, and software packages for general-purpose applications. It is, therefore, essential to complement efforts in software development with a comprehensive literature on new and existing methods, readily accessible to graduate students and researchers with an interest in current advances in the field.

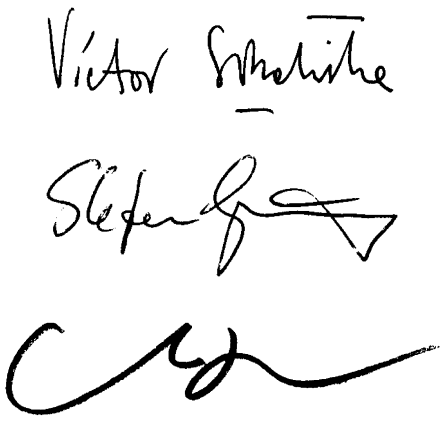
Victor S. Batista received his Lic. Ciencias Quimicas degree from Universidad de Buenos Aires, Argentina (1989) and a Ph.D. in Theoretical Chemistry from Boston University (1996). He also received the Sugata Ray Award from Boston University (1995) and completed postdoctoral fellowships with William H. Miller at the University of California, Berkeley (1997–1999) and Paul Brumer at the University of Toronto (2000). In 2001, he joined the Yale faculty as an Assistant Professor. He was Associate Professor of Chemistry (2005–2008), and Director of Undergraduate studies (2008–2010). In 2008, he was promoted to Full Professor with tenure. He is currently Senior Editor of the Journal of Physical Chemistry C.

Stefan Grimme studied Chemistry in Braunschweig and finished his Ph.D. in 1991 in Physical Chemistry on laser spectroscopy. He did his Habilitation in Theoretical Chemistry in the group of Sigrid Peyerimoff. In 2000 he obtained the C4 chair for Theoretical Organic Chemistry at the University of Münster. In 2011 he accepted an offer as the head of the newly founded Mulliken Center for Theoretical Chemistry at the Universtity of Bonn.

Markus Reiher has been Professor for Theoretical Chemistry at the Laboratory of Physical Chemistry at ETH Zurich since 2006. Before this appointment he had been working at the Universities of Jena, Bonn, Erlangen, and Bielefeld and he was a visiting researcher in Tromso, Budapest, Tel Aviv, Lund, and Singapore. His main research fields are relativistic quantum chemistry, electron-correlation theories, transition metal chemistry, and vibrational spectroscopy.

The present issue of *ChemPhysChem* is devoted to recent progress in a wide range of areas of Theoretical and Computational Chemistry by world-leading experts, reflecting the broad scope and rapid development of the field. For example, methodological developments for the treatment of excited states, heavy element systems, and non-covalent interactions are included. Another main topic is the computation of spectroscopic properties such as Raman optical activity, hyperfine coupling constants, NMR parameters or two-photon absorption intensities. The computation of these more complex properties has emerged as a research area that is of outstanding importance for the interpretation of modern spectroscopic experiments. Many of the applied papers in this issue furthermore reflect a current trend to model multicomponent systems of increasing complexity. The theoretical treatment of such inorganic/organic/bio-hybrids, which often include phase boundaries and require descriptions with periodic-boundary conditions, needs new approaches for the description of the basic electronic structure and for handling a huge number of degrees of freedom—some of which have already been proposed.

This issue of *ChemPhysChem* reflects all these developments and we hope that the reader will find this selection useful, enjoyable and stimulating for her or his own work.



Received: October 28, 2011

