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# EDITORIAL

This issue dedicated to Computational Chemistry in Switzerland is a most timely one for two reasons. First, we shall host in Geneva, September 11–15, 2005, a congress which is generally considered as one of the most important in the world by the community of developers and practitioners of Density Functional Theory (DFT), namely the 11th International Conference on the Applications of DFT in Chemistry and Physics (DFT2005). Undoubtedly, CHIMIA is the ideal journal to publish the final conference program together with all the abstracts of the invited lectures, oral contributions, and posters which will be presented during DFT2005. Second, we thought that it was relevant to include in the same issue as well a selection of articles written by distinguished computational chemists active both in Swiss academia and industries so as to enlarge the range by offering to the readership of CHIMIA a broad panorama of this rapidly evolving discipline. Of course, to have a scope for this issue as large as possible, the articles presented in this second part relate to various and complementary topics of computational chemistry and not necessarily to DFT.

Computational chemistry has become an indispensable partner of experiment. Among numerous applications, it may be used to model complex systems, with applications such as rational drug design, selection and synthesis of new materials, and modeling of environmental processes. In this context, quantum chemistry is the method of choice when information related to electronic structure or, more generally, when parameters of classical methods are not available. Among the most widespread methods of quantum chemistry, DFT has made a remarkable breakthrough in the last few years. Today, DFT methods have become *de facto* the standard techniques for modeling organic, inorganic and organometallic systems, clusters, catalysts, new materials, surfaces, *etc.* In addition, on the scene of the DFT methodology itself, important advancements may be predicted in the next few years in view of the considerable efforts spent worldwide.

Since 1984, biennial international conferences devoted exclusively to DFT have been organized in Europe. The 11th Conference, DFT2005, will thus take place from September 11 to 15, 2005, in Geneva. This Conference succeeds previous ones organized in Brussels (2003), Madrid (2001), Rome (1999), Vienna (1997), *etc.* The main purpose of DFT2005 is to report state-of-the-art developments, both in methodology and applications, carried out in chemistry and physics. In particular, the Conference is aimed at a wide coverage of DFT quantum chemistry as well as of collaborations involving activities outside the field itself. Indeed, the last half of the 20th century has seen an accelerating and impressive growth in the capability and scope of quantum chemistry, in particular of DFT, with the award of the 1998 Nobel Prize to John Pople and Walter Kohn. Let us emphasize here that the latter, generally considered as the 'father' of DFT, will be an invited speaker of DFT2005.

We are proud that Switzerland and Geneva have been chosen to host this prestigious Conference. On behalf of both the Local and At-Large Organizing Committees, it is our pleasure to welcome all the participants to DFT2005. We are particularly delighted by the interest the Conference has aroused among the DFT community and much beyond. To a great extent, such a large response is undoubtedly due to the variety of topics covered and to a judicious choice of eminent lecturers. We thank all of them, and our sponsors as well, for making possible this event, for which all the ingredients are there to be a success.

Finally, as mentioned above, this issue is also intended to present a broad panorama of computational chemistry as practiced in Swiss academia and industries. To this end, eleven articles are presented with the aim to cover the most

relevant applications of this well-recognized discipline. Of course, the selection we made of potential authors is somewhat arbitrary and far from being exhaustive. Our main purpose was to show how varied the activities in this field can be in the context of chemistry, physics, and the life sciences. The reader will thus discover some major and innovative developments carried out, both as far as methodology and applications are concerned in electronic structure of molecules and atoms in condensed phase, photochemical processes in complex environments, ground- and excited-state properties of transition metal complexes, binding energies of hydrogen-bonded systems of biological interest, energetics and dynamics of photodissociated CO and NO in myoglobin, interplay between experiment and theory in solving problems associated with reactive intermediates, parity violation in chiral molecules, DFT applications to systems comprising several thousand atoms, selection of the best candidates in drug discovery, computational applications in life sciences industry, and the concept of electron delocalization in organic chemistry. Here again, we are much indebted to the authors of these articles for having accepted our invitation and for their significant contribution to the advancement of computational chemistry in Switzerland.

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