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International Journal of
**QUANTUM
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An
Interview with
Peter R. Schreiner

Quantum
Chemistry
Reloaded

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Interview with Peter R. Schreiner

Editor of the Journal of Computational Chemistry

Editor-in-Chief of WIREs Computational Molecular Science

Q: You are the Editor of both JCC and WIREs:CMS. What is your vision for the two journals in the coming years?

First of all, the two journals serve different purposes. JCC is a regular original research journal that reports on the newest and hottest developments in the field, in publication formats such as rapid communications, original articles, selected reviews as well as software news and updates. WIREs:CMS on the other hand is a new publication medium as it bridges the gap between a classic encyclopedia (like its print predecessor, the highly successful *Encyclopedia of Computational Chemistry*) and a regular review journal that come in the formats of overviews (for relatively new topics) and advanced reviews (for well-established research directions). Additional article types that allow more of a personalized flavor such as expressed in "opinion" articles and such aiming at topics that are just beginning to take shape ("focus" articles) plus software reviews complete the picture. The two journals cover essentially all publication formats and subject development stages. With the rapid development of computational chemistry, I believe this is a good "twin" strategy for authors to find the right format for their work and for the two journals to be able to continuously adjust to the current demands of their readers.

Q: Why did you decide to be so involved in scientific publishing, as journal editor?

There are several reasons. First, being a journal editor allows staying on top of the information chain regarding the most recent developments in a particular field. This is like being forced to doing "homework" by reading a lot of scientific articles from scientists around the world. One also gets a good feeling for new developments and the distribution of scientists working on particular sub-fields. The second motivation is my keen interest in scientific writing; describing new findings in clear words is always a challenge and I am continuously learning from the many excellent papers submitted to the journals I am involved with. Finally, I am firmly convinced that scientists, as opposed to journalists, should do science editing even though the language may not be the most refined (the two are not mutually exclusive, though!).

Q: Here in Lugano you are chairing the Evening Session on "The Role and Perspectives of Modeling and Simulation in Chemical and Pharmaceutical Research". Why computer modeling matters in industrial research?

Simple answer: cost. It takes about one billion Euros (currently about 1.3 billion US Dollars) to develop a drug from a promising drug candidate. Currently, projects are terminated at a late stage because of some unforeseen effects in late clinical phases. This is a disaster for the industry that aims at a scenario that "if you fail, fail early". Early failure means that one needs a wealth of information on a new drug including toxicology profiles, metabolism etc. As modeling and simulation is increasingly able to address these issues, it is imperative that these relatively cheap – as compared to late-stage clinical trials – approaches are used early and with full force to eliminate dead ends and to avoid exorbitant costs.

Q: What is the focus of your research right now, in a nutshell?

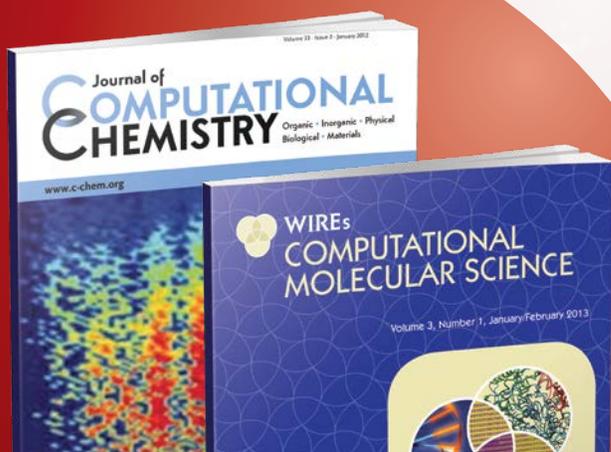
All of our work combines experiment with high-level theoretical approaches. We follow three research directions that all benefit highly from this fruitful interplay: a) organocatalysis (hereby seeking a mechanistic understanding through computational chemistry approaches, b) reactive intermediates (most of our attention focuses on tunneling reactions in organic chemistry – theory here is key to rationalize these hard to grasp quantum effects on reactivity), and c) nanodiamonds (which show beautiful London dispersion effects that I will be talking about in my scientific lecture).

Q: What inspired you, at the beginning of your career, to choose Computational Chemistry as your field of interest?

This is an easy one: my doctoral advisors, Paul Schleyer and Fritz Schaefer, because of their engaging personalities and their enthusiasm for computational chemistry. I also recognized computations as an analytical instrument like a spectrometer that you can use to learn more about molecular structures and properties. One can test new ideas more quickly with (simple) computations, even when you are far away from a lab. As a notoriously impatient person, this is a real advantage!



Dr. Peter R. Schreiner is Professor of Organic Chemistry at Justus-Liebig-Universität Giessen, Germany and an Adjunct Professor at the University of Georgia, USA.



Professor Peter R. Schreiner will be chairing the Evening Session on "The Role and Perspectives of Modeling and Simulation in Chemical and Pharmaceutical Research" on Wednesday, June 5th (18:00) at the Università della Svizzera italiana, Auditorium AZ. His talk at MQM-2013 is on Tuesday, June 4th at 15:00.

Quantum Chemistry Reloaded

When Per-Olov Löwdin founded the *International Journal of Quantum Chemistry* in 1967 quantum chemistry was entering the modern era, beginning to explore the potential of computers as well as extending its realm beyond the study of atoms and molecules to small systems of biological interest. Löwdin's vision for the discipline is reflected in his editorial for the inaugural issue of the journal.^[1] Coming into existence through the interactions of physics, chemistry, applied mathematics, and what we now would call computer science, modern quantum chemistry has been a naturally interdisciplinary field from the outset, and *IJQC*'s role is to report and facilitate this interplay of theory, computational algorithms, and applications to atoms, molecules, crystals, and biology, in close connection with experiments.

In the nearly half a century since that historic editorial, quantum chemistry has experienced continuous evolution, harvesting the most exciting developments from the parent fields. The rise of materials science research, for example, has brought the challenge of extending the predicting power of quantum chemical calculations to ever larger and more complex systems, whereas the study of chemical reactivity and biological processes requires the accurate simulation of atomic dynamics by first-principles. In the same way, the introduction and optimization of new, powerful, and sophisticated spectroscopic techniques calls for increasingly accurate theoretical approaches for their interpretation, and computational algorithms and software must be developed to adapt to new, ever more powerful computer architectures: from massive parallel supercomputers with hundreds of thousands of processors to systems based on graphical chips. Finally, the application of quantum information concepts to chemistry^[2] could drive a new beginning for quantum chemistry, similar to that experienced with the advent of electronic computers 50 years ago.

Mirroring quantum chemistry's path, *IJQC* must also evolve to continue to serve its original mission of fostering the exchange of ideas between researchers from all aspects of the discipline.

A journal at the service of today's quantum chemistry community demands modern publishing processes, and we have been working hard to improve our manuscript handling and production procedures to ensure that your research is available to the community as soon as possible. These efforts have resulted in the reduction of the acceptance to online publication time to a very competitive 15 working days on average. Our team of professional in-house editors is focused on delivering rapid and rigorous peer-review, keeping well in sight the journal's role in **providing interdisciplinary communication and scientific insight**, and not just simple numerical results. With our **new Reviews and Tutorials series**,^[3] we plan to echo the versatility and variety of modern quantum chemistry, and by making these articles free to access we hope to give everybody an opportunity to discover new aspects of this stimulating discipline. Moreover, our most exciting articles are now highlighted through the very popular **ChemistryViews.org** and **MaterialsViews.com**, Wiley's chemistry and materials science news sites, to guarantee them the great exposure they deserve even beyond the theoretical chemistry community. Finally, we hope that you have already appreciated *IJQC*'s new look, which premiered last year with issue 17/2012. In addition to full-page cover images, highlighting some of the most interesting articles of every issue, we have introduced a graphical table of contents to guide you quickly to the papers of your interest in the journal, both online and in print.

We look forward to what the future holds in store for quantum chemistry. Whatever this may be, you will read it on the pages of *IJQC*.

Enjoy the "reloaded" *International Journal of Quantum Chemistry*!

Matteo Cavalleri

Editor-in-Chief, *International Journal of Quantum Chemistry*

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1 P. O. Löwdin, *Int. J. Quantum Chem.* 1967, 1, 1.

2 B. P. Lanyon, J. D. Whitfield, G. G. Gillett, M. E. Goggin, M. P. Almeida, I. Kassal, J. D. Biamonte, M. Mohseni, B. J. Powell, M. Barbieri, A. Aspuru-Guzik, A. G. White, *Nature Chem.* 2010, 2, 106.

3 <http://reviews.q-chem.org/>, <http://tutorials.q-chem.org/>

This page has previously appeared as an Editorial in the *International Journal of Quantum Chemistry* 113:1 (2013).

Virtual issue

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