ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

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IBM

# C4 WORKSHOP

# COMPUTATIONAL QUANTUM CHEMISTRY: QUO VADIS ?

## THURSDAY, JUNE 8, 2017

## ETH ZURICH

## AUDITORIUM HCI G3

### THE WORKSHOP

Modeling and simulation are well established tools in virtually all areas of chemical research. Once a niche for a few enthusiasts, computational chemistry has gained tremendous momentum and it is not always clear which way the discipline will go: many new methods are being presented, writing software has turned into an art in its own right, and novel, possibly disruptive types of hardware enter the scene. Finally, approaches such data-driven modeling call for our attention.

The goal of the Workshop, hosted by the Laboratory of Physical Chemistry of ETH Zürich, is to put these developments into proper perspective and to find answers to the question of the directions computational chemistry may take in the near future. The invited speakers will address different aspects, including the relationship with experiment. Finally, the different scenarios will be visited in a panel discussion.

After the panel discussion, an Apéro will be served to continue the discussion among all participants. This workshop also is a farewell to Dr. Hans Peter Lüthi, chairman of the C4 Steering Committee, who will retire from ETH Zürich after thirty years of service.

## THE PROGRAM

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| 10:00 – 10:10 | Jürg Hutter<br>*Welcome Address* |
| 10:10 – 10:30 | Hans Peter Lüthi<br>*A Brief Look Back* |
| 10:30 – 11:00 | Samuel Leutwyler<br>*Connecting Experiment and Theory:*<br>*Marriage has Many Pains, but Celibacy has no Pleasures* |
| 11:00 – 11:30 | Hiroko Satoh<br>*QM-based Data Chemistry: PES-based Automatic Deduction of Conformational Transition Networks at the Quantum Mechanical Level* |
| 11:30 – 12:00 | Peter A. Limacher<br>*The Advent of Single-Reference Methods in the World of Multi-Reference Problems* |
| 12:00 – 13:30 | Lunch Break |
| 13:30 – 14:00 | Wim M. Klopper<br>*Using the GW and Bethe-Salpeter Methods in Molecular Quantum Chemistry* |
| 14:00 14:30 | Trygve U. Helgaker<br>*Density Functional Theory in Ultrastrong Magnetic Fields* |
| 14:30 – 15:00 | Coffee Break |
| 15:00 – 15:30 | Sabre Kais<br>*Near Term Applications of Small Scale Quantum Computing* |
| 15:30 – 16:00 | Alessandro Curioni<br>*Title to be announced* |
| 16:00– 16:15 | Intermission |
| 16:15 – 17:00 | Panel Discussion<br>*Computational Quantum Chemistry:Quo Vadis?*<br>Moderator: Markus Reiher<br>Panelists:<br>W.M. Klopper, T.U. Helgaker, S. Kais, and A. Curioni |
| 17:00 – 18:00 | Apéro |

## THE SPEAKERS / PANELISTS*

**Alessandro Curioni*,** trained as theoretical chemist at the Scuola Normale Superiore in Pisa, was recently appointed as director of the IBM Research Laboratory in Rüschlikon. Before, he was the head of the Cognitive Computing and Computational Sciences Department of IBM Research. His work on high-performance computing and computational science targeted scientific and technological problems in several industries including healthcare, consumer goods and electronics. He is also leading the research activities for the newly established Watson Internet of Things unit.

**Trygve U. Helgaker*** is a professor of chemistry at the University of Oslo and director of the Norwegian Centre for Theoretical and Computational Chemistry (CTCC). His research is focused on the development of efficient computational methods for large molecular systems, containing hundreds of atoms. Working on the fundamentals of density functional theory, his goal is to make studies on large systems as accurate as those on small and medium-sized systems. He is also a developer of the DALTON codes.

**Sabre Kais***, who received his degrees from Hebrew University, is a professor of chemical physics at Purdue University, also holding courtesy professorship appointments at the Departments of Computer Science and Physics. He is also the Research Director of the theory group at the Qatar Environment and Energy Research Institute. His research focuses on electronic structure and dynamics of finite systems, quantum criticality, dimensional scaling and quantum information and computation.

**Wim M. Klopper*** has the chair of theoretical chemistry at the Karlsruhe Institute of Technology (KIT). He developed wave function based methods containing two-electron components, and is one of the authors of the TURBOMOLE program package. His applied research agenda also covers subjects such as soft matter and functional materials. After his PhD (Bochum) and post-doctoral studies (University of Minnesota), he worked with H. P. Lüthi at the ETH Zürich Interdisciplinary Project-Center for Supercomputing.

**Samuel Leutwyler** is a professor at the Department of Chemistry and Biochemistry of the University of Bern. Exploring structures, vibrations and energetics of van der Waals and hydrogen-bonded complexes by means of UV and IR laser spectroscopy, theory and quantum chemical modeling were important complementary tools in his research. For that matter, he had an intense collaboration with W. Klopper and other leaders in the field.

**Hans P. Lüthi** started his career in computational quantum chemistry as an IAESTE scolar hosted by Jan Almlöf in Oslo testing the MOLECULE-SWEDEN MC-SCF codes on the rotational barrier of ethylene. Getting most out of a computational infrastructure let to the introduction of the direct Hartree-Fock method and its parallelization all the way to global networks of (parallel) computers. Later, his focus turned to “doing real chemistry”, i.e. the prediction of the molecular properties and reactivity of carbon-rich compounds, weakly interacting systems and reagents.

**Peter A. Limacher** was a PhD student with H.P. Lüthi at ETH Zürich. After post-doctoral studies at McMaster University with P. Ayers, he is now working with W. Klopper in Karlsruhe. His research interest is in the development of highly efficient and accurate wave-function based quantum chemical methods.

**Hiroko Satoh** is a professor at the Research Organization of Information and Systems (ROIS, Tokyo, Japan) and a researcher at the Department of Chemistry of the University of Zurich. Her main research interests are in the areas of chemoinformatics and computational chemistry. She visited ETH Zürich from 2007-2008 hosted by H.P. Lüthi and started a joint project on QM-data centric chemistry. Since 2008, she has conducted a project on molecular- and reaction discovery based on automatic global reaction route mappings (GRRM).

## PARTICIPATION

Those interested in participating in the workshop are kindly requested to send a note to c4@phys.chem.ethz.ch confirming their attendance. Participation is free of charge.

## THE C4 WORKSHOP ORGANIZERS

Profs. Markus Reiher (ETH Zürich), Jürg Hutter (Universität Zürich), Alessandro Curioni (IBM Research) and PD Hans P. Lüthi (ETH Zürich)