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Conference Report

Symposium of Theoretical Chemistry in Zurich

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In September 2023, the Symposium of Theoretical Chemistry (STC) was held at ETH Zurich. This was the 59th installment of the conference series held annually in Germany, Austria or Switzerland, although it had not previously been held in Zurich since 1966. This year's event was organized by ***Sandra Luber*** (Univ. Zurich) and ***Jeremy Richardson*** (ETH Zurich) with a focus on quantum and classical dynamics in chemistry.

The lectures were held in the Audi Max in ETH Zurich's main building and were opened by ***Michele Parrinello*** (Italian Institute of Technology Genoa), who presented recent work on simulating the Haber–Bosch cycle. He explained how the surface of the catalyst restructures itself in the presence of the N_2 reactant. In addition to the scientific insights gained, the audience were entertained by movies of the dancing atoms accompanied by music. Following this were two shorter talks from ***Bartosz Blasiak*** (Univ. Frankfurt), who discussed quantum simulations of large amplitude motion in a protonated Schiff base, and ***Sophia Bazzi*** (Univ. Göttingen), who presented her discovery of rare N–O–S bonds in proteins.

After a coffee break to catch up with old friends, ***Ali Alavi*** (MPI for Solid State Research) opened the next session and explained how transcorrelation could be used to evaluate high-level electronic-structure calculations more efficiently, also using a new approximation (xTC) to the three-body interactions. In particular, he showed how to overcome the problems of having non-Hermitian matrices. ***Roberto Marquardt*** (Univ. of Strasbourg) presented an intriguing set of results about the quantum nature of the mean-square displacement, and ***Giovanni Li Manni*** (MPI for solid state research) explained how to tackle poly-nuclear transition metal clusters using spin symmetries and the strategy of Quantum Anamorphosis for strongly correlated electronic states.

A poster session brought the first day to a close, with over 100 posters. The participants were refreshed by an apéro to help their discussions continue in the busy environment until late in the evening.

The second day opened with the Hellmann award lecture. This prize is presented each year to a scientist under 40 without a permanent research position and the winner is kept a closely guarded secret until it is announced at the STC. This year, the award went to ***Carolin König*** (Univ. Hannover) for her work on vibrational spectroscopy. After a laudatio given by Markus Reiher, she explained how her work enables even large molecules to be treated accurately by vibrational analogues to electronic-structure methods. Following this, two former doctoral students, ***Ansgar Pausch*** (KIT) and ***Viktor Zaverkin*** (Univ. Stuttgart) were awarded the Peyerimhoff award for their excellent doctoral theses on the topics of molecules in strong magnetic fields and machine learning of potential energy surfaces, respectively. Note that any student who carries out their doctoral thesis in Germany, Austria or Switzerland in the field of theoretical chemistry can apply for this award, and female applicants are particularly encouraged as they have been under-represented in the list of applicants.

Hellmann and Peyerimhoff award ceremony.

The day continued with talks from ***Trygve Helgaker*** (Univ. Oslo) on magnetic fields so strong that they can make all four H atoms in a methane molecule fan out on one side. This was followed by ***Konstantin Gaul*** (Univ. Marburg) who studied how parity-violation could modify a molecule's equilibrium structure and presented a proposal for how this could be measured with rotational spectroscopy. As the next speaker was unable to attend due to illness, ***Joseph Lawrence*** (ETH Zurich) stepped in at the last minute to present his work on computing accurate tunnelling splittings using instanton theory with perturbative corrections.

Over 300 participants attended, a record for an STC held in Switzerland.

Prof. Helgaker presenting his lecture.

The next session was opened by Angel Rubio (MPI for the structure and dynamics of matter), who introduced the audience to cavity quantum electrodynamics effects in chemistry and discussed the design of Floquet states of matter. This was followed by ***Lukas Lang***'s presentation (TU Berlin) on how to recover the usual chemist's understanding of molecular structure when presented with a many-body wavefunction in which all nuclei are completely delocalized and spherically symmetric. ***Roman Ovcharenko*** (LMU Munich) then introduced an efficient method for implementing the quasi-adiabatic path integral method for propagating dissipative quantum dynamics exactly in system-bath models.

For some of us the day continued with the annual general meeting of the Arbeitsgemeinschaft Theoretische Chemie (AGTC) in which, among others, Christoph Jakob and Benjamin Schröder informed about the NDFI4Chem initiative, leading to a thought-provoking discussion of how electronic data could be better shared among theoretical groups. When we emerged from the meeting, a second poster session (with another 100 posters) was in full swing as the students were eager to start early without us.

The first session of the next day was dedicated to nonadiabatic dynamics. ***Federica Agostini*** (Univ. Paris Saclay) explained how trajectory-based methods can be used to simulate photochemistry and presented recent advances for the exact factorization approach. ***Daniel Bultrini*** (Univ. Heidelberg) discussed how in principle quantum computers could be used to simulate mixed quantum–classical dynamics, although hinted that on current quantum computers, this would not yet be efficient. The final talk was given by ***Jonathan Mannouch*** (MPI for the Structure and Dynamics of Matter), who presented a mapping approach to surface hopping and showed simulations where the results are more accurate than the standard surface hopping method.

In the next session, ***Thomas Bondo Pedersen*** (Univ. Oslo) spoke about time-dependent coupled cluster methods for simulating attosecond dynamics such as the proper choice of orbitals and design of laser pulses, and ***Elke Fasshauer*** (Univ. Tübingen) presented a theory for interparticle Coulombic decay. The final talk was given by ***Bettina Keller*** (FU Berlin), who showed how to sample rare events using Girsanov reweighting.

The afternoon was left free for the participants to explore Zurich or join offered activities. Despite the forecast of light rain, many participants climbed the Uetliberg or went swimming. Others visited the Kunsthaus or took a boat ride on the Zurich lake. In the evening, we sat down to a dinner together, held in the ETH main building.

On the final day, ***Ivano Tavernelli*** (IBM Research) gave an introduction to quantum computing from the perspective of quantum chemistry and showed algorithmic developments such as embedding techniques for combining quantum electronic structure algorithms with density functional theory. ***Jakob Kottmann*** (Univ. Augsburg) followed with novel approaches for designing quantum circuits. Finally, another late cancellation allowed ***Benjamin Stamm*** (Univ. Stuttgart) to present his work on speeding-up simulations using a better initial guess for the self-consistent field procedure.

The final session was opened by ***Mariana Rossi*** (MPI for the Structure and Dynamics of Matter), who discussed simulations of molecules on metal surfaces and the importance of friction. ***Johannes Tölle*** (Caltech) then presented efficient methods based on GW theory which could tackle electronic-structure problems as large as $C_{50}H_{102}$. The honour of being the final speaker was given to ***Joseph Subotnik*** (Univ. Pennsylvania), who discussed the enigma of chiral-induced spin selectivity. He proposed that the effect emanates from an elusive force derived from the Berry connection.

At the end of the meeting, six poster prizes were awarded to ***Marit Fiechter*** (ETH Zurich), ***Niclas Krupp*** (Univ. Heidelberg), ***Paolo Lazzaroni*** (MPI for the Structure and Dynamics of Matter), ***Jessica Meyr*** (Univ. Würzburg), ***Bonasree Roy*** (Univ. Potsdam) and ***Lisamaria Wallner*** (Univ. Heidelberg), who all received a box of Sprüngli chocolates as well as prize money from the AGTC.

The poster prize winners and organizers.

Overall, we were very happy to be able to host the community in Zurich and hope that all participants enjoyed the symposium and left with a good impression, as it is through events such as these that Swiss institutions can keep their high standing in the academic world and attract the best students and researchers. Next year the STC will be held in Brauschweig, hosted by Christoph Jakob and Jonny Proppe.

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