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Conference Report

PTPC2019: Photon Tools for Physical Chemistry 2019

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The Photon Tools for Physical Chemistry (PTPC) meeting was held on 8–11 January 2019 at Hotel Dorint Blüemlisalp in Beatenberg, bringing together 63 participants from 12 countries in four continents.

PTPC2019 followed in the footsteps of the previous PTPC2014 meeting and intended to broaden the scope of past events held at Lund (2010), Shanghai (2011), and Argonne (2013) to include novel light sources, such as free electron lasers, and their application in physical chemistry.

The meeting covered a broad spectrum of topics ranging from molecular dynamics, spectroscopy, catalysis, astrochemistry, combustion, and kinetics to the characterization of nanoparticles and aerosols with photon tools. Time-resolved experiments from microsecond to femtosecond time scales were shown to yield direct insights into processes ranging from charge transfer in photovoltaics to combustion. The topics also included the photochemistry of excited states and the quest to find the origin of interstellar molecules, most notably polycyclic aromatic hydrocarbons. Spectroscopic interrogation techniques were discussed to study reaction dynamics in the gas phase and state-selected reactivity on surfaces, to understand particulate matter, and to unveil reaction mechanisms in harsh environments.

The ultimate goal of the meeting was to establish and promote synergies and tackle topical issues in physical chemistry using state-of-the-art IR, VUV, and soft X-ray synchrotron and free electron laser radiation as well as lab-based sources. The conference program consisted of 12 sessions on the following nine themes: Time-resolved techniques, New opportunities, Nanoscale aggregates, Surfaces and catalysis, Astrochemistry, Combustion and flame, Spectroscopy in action and action spectroscopy, Photoionization spectroscopy, and Reaction kinetics and mechanisms. During the talks and discussions, professors, senior researchers and the next generation of scientists could exchange knowledge and ideas face-to-face. The 50 speakers came from a broad background, and, among them, 16 were PhD students and postdocs.

In his keynote address, ***Kiyoshi Ueda*** presented ultrafast electronic and nuclear dynamics experiments at SACLA showing deep inner-shell photoionization and multiple electronic decay cycles in Xe[1] and discussed the mechanism of ultrafast Coulomb explosion in diiodomethane.[2] In the following, we would like to refer to ten further highlights to illustrate the breadth of contributions. ***Christoph Bostedt*** introduced the free electron laser at Paul Scherrer Institute, SwissFEL,[3] including future development plans. ***Daniela Rupp*** explained how free electron laser radiation from FERMI and neural networks unveiled the three-dimensional shapes of spinning helium nanodroplets.[4] ***Ruth Signorell*** showed how one can rely on the thorough description of electron scattering processes in nanoparticles[5] to obtain the genuine binding energy of the hydrated electron.[6] ***Gerd Ganteför*** introduced a new magnetic bottle electron trap photoelectron spectrometer to the audience, to be used in electronic structure studies of metal nanoparticles.[7] ***Jeroen van Bokhoven*** and co-workers used *in situ* X-ray absorption spectromicroscopy to study catalyst support effects on the surface migration of hydrogen atoms (hydrogen spillover).[8] ***Katharina Kohse-Höinghaus*** discussed the current and future challenges facing combustion chemistry.[9] In order to understand high-pressure reactive environments, novel approaches have to be developed to probe these directly. ***Leonid Sheps*** described such an experiment, which revealed, *e.g.*, the pressure-dependent competition among reaction pathways in tetrahydrofuran oxidation.[10] ***Majdi Hochlaf*** *et al.* relied on single photon ionization slow photoelectron spectroscopy to identify cytosine isomers in the gas phase.[11] ***Frédéric Merkt*** explained how apparently irreconcilable differences between the most accurate experimental and theoretical hydrogen molecule dissociation energies may in fact hint at a revised proton charge radius or an improved value of the proton-to-electron mass ratio.[12] Finally, ***Judit Zádor*** presented an automated potential energy surface exploration tool, KinBot, to help kineticists find crucial transition states and understand reaction mechanisms *in silico*.[11]

The conference was well received: "Many thanks for organizing such a beautiful meeting that I really enjoyed. I found that our broad field has now reach a very high level of quality and maturity.", "Thanks again for organizing this very nice meeting – it was very interesting and I believe a great success!" Thus, the organizing committee, together with the local organizers from the Paul Scherrer Institute, succeeded in compiling an inspiring scientific program to bring together researchers and, hopefully, to initiate successful collaborations.

The organizers gratefully acknowledge the backing of the Paul Scherrer Institute, the Swiss Federal Office of Energy, and Pfeiffer Vacuum. Financial support from the latter two sponsors enabled the participation of 10 PhD students and postdocs at a significantly discounted fee. The detailed program and abstracts are available at *https://www.psi.ch/sls/vuv/ptpc2019*

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