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Conference Report

XXII. Symposium on Atomic, Cluster and Surface Physics (SASP)

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Abstract: From Sunday February 2nd, 2020 until the following Friday, 75 scientists from all over the world gathered in Hotel Laudinella in St. Moritz to discuss their latest findings about surface, cluster and gas phase physics and chemistry. A program consisting of 25 invited speakers, 16 hot topic oral contributions and 27 poster presentations has been put together by the organizers from Empa.

The Symposium on Atomic, Cluster and Surface Physics (SASP) is a series of biennial international conferences, which seeks to promote the growth of scientific knowledge and effective exchange of information among scientists in the field of atomic, cluster and surface physics. The symposium deals in particular with collisional interactions involving different types of collision partners, *i.e.* electrons, photons, molecules, nanoparticles, and surfaces. Starting in 1978 in Italy, SASP takes now place every second time in Austria, from 2006 onwards in Obergurgl. The respective following events have switched between Italy, France and Switzerland (Engelberg 1996, Les Diablerets 2008, Davos 2016). Throughout the years SASP has become a truly global conference, with participants from the US and Canada, China, Japan and all over Europe. In 2020 it was time to return to Switzerland, so the attendees headed for St. Moritz in early February. Beyond the below-detailed invited lectures, state-of-the-art science was presented in several contributed, so-called hot topic talks. Ample time was allocated to free discussions (Fig. 1) and two evening poster sessions (Fig. 2).

Fig. 1. Outdoor scientific discussions above St. Moritz.

After arrival and registration on a sunny Sunday in snow-covered Engadin valley, the crowd was welcomed by the conference chair (KHE), who stressed the importance of the financial support and acknowledged the sponsoring provided by the Swiss National Science Foundation (SNSF), the Swiss Chemical Society (SCS), Empa, the Royal Society of Chemistry (*Chem. Soc. Rev.*), as well as companies, such as Hiden, Tyracont, Specs, Zurich Instruments, Prevac, Radient Dyes, Scienta Omicron and Createc.

Fig. 2. Lively discussions evolved in two evening poster sessions during the week.

The Sunday night session after dinner took off with a talk by Nobel laureate ***Ben Feringa*** from University of Groningen. After the SAOG Meeting in Fribourg in 2019 and the Chirality@The Nanoscale meeting in Ascona in October (see Conference Report in CHIMIA 2019, 73, 1042–1043), it was the third time within 12 months that he could join us in Switzerland for a scientific meeting. This time he focused on 'Molecular Switches and Motors at Interfaces' and presented propulsion of molecules on surfaces (nanocar) and how materials systems, such as polymers and liquid crystals can be altered by light-induced unidirectional molecular rotation. The next speaker, ***Jochen Küpper*** from Desy in Hamburg, showcased that strong laser fields may influence molecular alignment, induce controlled molecular rotation as well as state-selected ionization and diffraction of photoelectrons.

The structure of insulin at the water–air and water–solid interfaces was the topic of the first talk on Monday morning by ***Heike Arnolds*** from University of Liverpool. Using a range of vibrational spectroscopies, she showed that hydrophobic interfaces can actually stabilize the native structure of insulin and that unfolding only occurs well above room temperature. Bottom-up fabrication and electronic properties of atomically precise one- and two-dimensional nanoporous networks was the topic of ***Sabine Maier***'s (FAU Erlangen) presentation. Such structures can be synthesized by clever on-surface chemistry and were analyzed with scanning tunneling microscopy (STM) and density functional theory (DFT). By means of laser quantum state-resolved preparation of methane, its dissociation on nickel and platinum surfaces has been studied by the group of ***Rainer Beck*** from EPFL. He showed that the dissociation probability is site-specific and varies for terraces, steps and kink surface sites.

As first speaker of the Monday afternoon session, ***Wolf Widdra*** from Martin-Luther-Universität Halle-Wittenberg discussed lattice vibrations of perovskite and oxide surfaces and special phonon-polariton modes, arising from coupling of bulk-like phonons and surface electromagnetic waves. He was followed by ***Hans-Peter Steinrück*** from FAU Erlangen, who emphasized

ionic liquid/solid interfaces, studied in ultrahigh vacuum with X-ray photoelectron spectroscopy. He showed that rapid ion exchange processes lead to enrichment effects at the vacuum/liquid and the liquid/solid interfaces.

Fig. 3. Franz Giessibl, inventor of the tuning fork atomic force microscope, lectures on interactions between single atoms.

The Tuesday morning session was commenced by ***Franz Giessibl***, who described in detail atomic force microscopy with a carbon monoxide modified tip (Fig. 3). He demonstrated that this tool allows imaging of iron clusters with unprecedented resolution.

Meike Stöhr of Zernike Institute of the University of Groningen discussed structural and electronic properties of functional molecules on graphene/copper surfaces. By adding Cu adatoms, her group was able to establish metalorganic networks. Stereodynamics in mixed molecular beams of metastable neon and other rare gases and N_2 or CO (X) studied at sub-Kelvin temperatures was reported by ***Andreas Osterwalder*** from EPFL. He pointed out that the branching ratio to either $NeX^+ + e^-$ or $Ne + X^+ + e^-$ can be controlled by pre-alignment of the reactants.

The afternoon session took off with ***Alec Wodtke*** from Max Plank Institute for Biophysical Chemistry and University of Göttingen, who showed that laser excitation of CO molecules adsorbed on a NaCl surface transfer in part energy to other molecules into higher excited vibrational states, which were detected by infrared fluorescence with a new super-conducting single-photon detector. In his lecture, ***Leonhard Grill*** from University of Graz discussed single molecular motion on surfaces. By excitation by inelastic electron tunneling or photoisomerization, different switching and directional movements of various molecules was studied by STM.

Wednesday morning was devoted to recent progress in theory. ***Peter Saalfrank*** from University of Potsdam described different theoretical treatments of photo-induced surface processes, such as desorption and diffusion, by using DFT-based *ab initio* molecular dynamics including electronic friction in the non-adiabatic regime. Nuclear dynamics and sampling potential energy surfaces of flexible molecules and the role of tunneling in intramolecular hydrogen transfer were subject of the lecture given by ***Marianna Rossi*** from the Fritz Haber Institute (FHI) of the Max Planck Society in Berlin. By DFT-based structure search, she stressed how environmental changes, such as surface or charge, will reorient the chiral center of the amino acid arginine, for example. ***Martin Quack*** of ETH Zurich discussed parity violating energy differences between the ground states of enantiomers, which are in the range of 10^{-15} electron volts. Moreover, he proposed promising chiral candidates as well as experimental approaches to measure parity violation.

The afternoon session on Wednesday focused on experiments with ionic species in the gas phase. ***Juraj Fedor*** from the J. Heyrovský Institute of Physical Chemistry of the Czech Academy of Sciences presented his results on electron capture experiments with SF_6, which is widely used as insulator gas in high voltage devices. Due to its high greenhouse gas properties, he also presented experiments with alternative gases. Infrared spectroscopic studies performed with the free electron laser FELIX of the Radboud University in Nijmegen on small gas phase cations held in a cryogenic ion trap were presented by ***Sandra Brünken***. She unraveled isomer-selective reaction kinetics with species relevant in interstellar chemistry.

The Thursday morning started with a lecture on photoinduced phase transitions by ***Julia Stähler*** from FHI Berlin. She showed that the semiconductor ZnO turns metallic at its surface under intense laser pulses and decays back at femto- and picosecond timescales. Oxidation and reduction of gold electrodes during electrochemical water splitting, investigated with near-field *operando* Raman spectroscopy, was the subject of the contribution of ***Katrin Domke*** from Max Planck Institute for Polymer Research in Mainz. Her approach revealed valuable new insights into reaction intermediates and site-selective reactivity. Chiral metal clusters stabilized by thiolates were discussed by ***Thomas Bürgi*** from University of Geneva. That these represent stable but dynamic entities became evident by metal exchange between different clusters.

Fig. 4. Tuning properties of single atoms with the STM tip: Professor Franke talks about exploration of spin states on superconductor surfaces.

In the first afternoon talk, ***Katharina Franke*** of Freie Universität Berlin showed that coupling of transition metal atoms with super-conducting substrates will lead to spin excitations and may create so-called Shiba bands as well as topological states (Fig. 4).

The performance of carbon nanomembranes for water filtration, produced from molecular monolayer by radiation-induced crosslinking, was discussed by ***Armin Gölzhäuser*** of Bielefeld University. He showed that such membranes only allow water to pass, holding back basically all ionic species.

On departure day, ***Julia Kunze-Liebhäuser*** of University Innsbruck compared the performance of electrodes made from transition metal carbides with common copper electrodes for electroreduction of water and carbon dioxide. Mo_2C electrodes were characterized with photoelectron spectroscopy and Fourier transform IR spectroscopy, while gas products were tracked with differential electrochemical mass spectrometry and gas chromatography. Highly charged ions and their neutralization dynamics in 2D materials is one of the research themes treated by ***Friedrich Aumayr*** from TU Wien. He discussed, for example, the electron emission from single-layered graphene after impact of Xe^{30+} ions with up to 170 keV kinetic energy.

The symposium concluded with the bestowal of the SASP Schrödinger Award to ***Frédérik Merkt*** from ETH Zurich (Fig. 5). In his laudatory speech, Martin Quack highlighted Merkt's achievements in the fields of high-resolution spectroscopy, Rydberg states and ion dynamics. In the following award lecture, Merkt presented studies of reactions of H_2^+ and He^+ with neutral molecules such as N_2, H_2, CH_3F, *etc.* at temperatures as low as 1 K.

Fig. 5. Frédérik Merkt, (middle) wearing the Schrödinger Medal (inset) that he received from Roland Wester (left, U Innsbruck), representing the SASP Advisory committee. Martin Quack (right) gave the laudatory speech.

In conclusion, as one of the last meetings before the Sars-Cov-2-induced lockdown, the 22nd SASP Meeting in St. Moritz brought together scientists active in gas phase and surface physics and chemistry (Fig. 6), two communities that are hardly joining each other on meetings otherwise. The organizers got very positive feedback from the participants and were urged by many to organize a SASP meeting again in the near future.

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Fig. 6. Attendees of the 2020 Symposium on Atomic, Cluster and Surface Physics (SASP) in St. Moritz.