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11th Young Faculty Meeting, 5th June 2018Justin O. Zoppe^{*a}, Sereina Riniker^{*b}, and Leo Merz^{*c}

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In the tradition of the previous meetings, this year's «Young Faculty Meeting» consisted of a day with lectures of six young faculty members covering a diverse range of research fields in chemistry together with talks and discussions focused on career advice. The meeting took place in the beautiful location of the Haus der Universität (Bern) and was organized by **Justin Zoppe** (University of Fribourg), **Sereina Riniker** (ETH Zurich) and **Leo Merz** (SCNAT).

After a round of introductions, the meeting was kicked off by Dr. **Emiliana Fabbri** (Paul Scherrer Institute, PSI) with an eye-opening talk about perovskite nano-electrocatalysts for water splitting. Motivations for her work are the Swiss Energy Strategy 2050 that calls for replacement of nuclear energy with renewables and the growing global need to store large amounts of renewable energy. Hydrogen fuel is the most promising source to meet current energy capacity demands, thus her main interest is the oxygen evolution reaction (OER), which occurs at the alkaline water electrolyzer anode. Dr. Fabbri and her group are developing new anode materials for low temperature electrolyzers based on metal oxide nanoparticles with high surface area. They use X-ray absorption spectroscopy (XAS) to elucidate local electronic and geometric structures of such nano-electrocatalysts during operation. She presented a simple modified Adams fusion preparation method for iridium oxide nanoparticles, for which they found an inverse correlation between size and OER activity. Moreover, using state-of-the-art flame spray synthesis and time-resolved XAS, Dr. Fabbri ultimately showed that these materials display dynamic self-reconstruction of their surfaces during the OER. In more detail, *operando* XAS experiments revealed the growth of self-assembled metal oxy(hydroxide) layers at the nanoparticle surface, leading to their outstanding performance. As a result of her work, she proposed that costs of alkaline water electrolyzers can be drastically reduced without hindering electrolysis cell performance by using these highly active nanocatalysts.

Switching gears from catalytic materials to chemical ecology, Prof. **Stephan von Reuss** (University of Neuchâtel) introduced the audience to small molecule signaling in nematodes. These roundworms are among the most abundant animals on the planet, and range from the model organism *Caenorhabditis elegans* to diverse parasitic species of considerable concern for human health and agriculture. Developmental plasticity and behavior of nematodes are regulated by ascarosides – glycolipids based on ascarylose linked to fatty acid-like side chains – that are highly conserved in nematodes. Research by Prof. von Reuss and his group focuses on the development of bioanalytical tools to explore ascaroside structures, biosynthesis, and functions in diverse species. Combining ascaroside-selective mass-spectrometric screens and NMR-based structure elucidation along with total

synthesis, his group can accurately determine chemical structures and provide material for functional characterization. Their research demonstrates that the structural diversity is much greater than previously anticipated, because, depending on the nematode species, ascarosides are selectively derivatized with moieties of different biogenetic origin. Prof. von Reuss explained that the ascarosides could be considered as a modular library of small molecule signals that integrate building blocks from diverse primary metabolic pathways including carbohydrate, fatty acids, and amino acid metabolism. Similar mechanisms for the combinatorial assembly of other complex secondary metabolites appear to be prominent in nematodes in general and are currently also investigated in his group.



After the break, Dr. **Alice Soldà** (TU Munich) who is currently presiding the European Young Chemists' Network (EYCN, www.eycn.eu) presented the goals and activities of the network. The EYCN was founded in 2006 and is a division of the European Chemical Sciences (EuCheMS) with 27 member societies including the Swiss Chemical Society (SCS). Chemists under the age of 35 who belong to one of the member societies become automatically members of EYCN. The EYCN spent the last years working towards promoting the exchange of knowledge, experience, new ideas and projects among young chemists coming from academia and companies all across Europe. The aims of the network are: (i) improving the visibility of chemistry, (ii) getting closer to people from outside the research field (such as industry, business and management) and (iii) supporting young chemists at the beginning of their career with awards and activities focused on developing soft-skills and expanding their possibilities. Moreover, every two years, the EYCN announce the Young Chemist Award (EYCA). The activities of EYCN include projects such as video and photography competitions for high-school students, the Young Chemists Crossing Borders exchange program (YCCB) in collaboration with the Young Chemists Committee (YCC) of the American Chemical Society, mentoring of applicants for the Marie Curie Fellowship and ERC Starting grants, and connecting young chemists with industry mentors via the Mobility Mentoring Portal. In March 2019, the EYCN will host the 2nd European Young Chemists' Conference (EYCheM) in Bremen, Germany.

Following up on a different note, Dr. **Aleix Comas-Vives** (ETH Zurich) presented the use of bonding analysis and *ab initio* molecular dynamics (MD) simulations to elucidate mechanisms in heterogeneous catalysis. The system of interest was the ruthenium (Ru) catalyst in the Fischer-Tropsch synthesis of hydrocarbons from CO and hydrogen. The reactivity of Ru nanoparticles was found to depend on the size of the particles, with smaller particles being less reactive. Depending on the type of the reaction site (flat or step-edge) of the Ru nanoparticles, the mechanism of CO activation is thought to be different. CO is absorbed on the surface of the Ru nanoparticles and bonds with the Ru atoms through electron donation and back-donation. Through static calculations and bonding analysis, Dr. Comas-Vives showed that the back-bonding is increased at step-edge sites compared to flat sites. The size-dependent reactivity of the nanoparticles could be explained by the decreased extent of back-bonding with small particles, which disfavors direct cleavage of CO. At step-edge sites and at low coverage, the direct cleavage of the CO bond is thus the preferred mechanism. Conversely, Dr. Comas-Vives showed *via ab initio* molecular dynamics that the preferred mechanism for the CO activation under real catalytic conditions is the hydrogen-assisted CO cleavage on both flat and step-edge sites. His group is furthermore investigating computationally several types of heterogeneous catalysts active in energy conversion processes such as single sites on amorphous supports, zeolites and especially oxide-supported nanoparticles.

Before the lunch break, Prof. **Wendy Queen** (EPFL) shared her interests in metal-organic frameworks (MOFs) for separations. She explained the extraordinary surface area characteristic of MOFs and that a world record for any porous material of $7000 \text{ m}^2 \text{ g}^{-1}$, the area of a football field, was attained by MOFs. Besides separations, other applications of MOFs include sensing, energy storage and conversion. She is motivated by the fact that 10–15% of global energy costs are spent for separations, *e.g.* distillation. Moreover, around 11% of the world population has no access to clean drinking water. Her group therefore concentrates on the synthesis, characterization and adsorption properties of MOFs, both in gas and liquid phases. She shared a remarkable example of a MOF/polydopamine (PDA) composite synthesized by her group, which exhibits high selectivity for a variety of heavy metals in contaminated water. The system is based on iron 1,3,5-benzenetricarboxylate (Fe-BTC), which possesses mesoporous cages of 25 and 29 Å in diameter and open metal coordination sites for internal surface functionalization with PDA. Not only is the Fe-BTC/PDA composite inexpensive and highly selective for heavy metals, such as Pb^{2+} and Hg^{2+} , it is reversible, brings water to drinkable levels in seconds, and offers record-breaking removal capacities. Her group is now actively working on developing other MOF composites for the selective extraction of other contaminants and high value commodities from wastewater, rivers, and the ocean.



The topics regarding career advice of this year's meeting were «Hiring and getting hired». The afternoon session was started by Dr. **Thomas Eichenberger**, former Head of the Office of Faculty Affairs at ETH Zurich. He shared with the young faculty his experiences and observations from more than 300 faculty hirings over 27 years at ETH Zurich. An important aspect to balance career planning and luck is a strong network, which can be strengthened through international collaborations and conferences, inviting guests and teaming up with young colleagues. To find positions, Dr. Eichenberger advised to look also beyond well-trodden paths. During an assistant professorship it is important to focus on what will promote the career, but also to become a good group leader and strengthen one's soft skills. Regarding job interviews, he recommended to submit only what is asked for, put a lot of thought into the cover letter, present ideas for the future rather than the past, stress supervision and teaching skills, and be ready for blue-sky questions. The topic of good group leadership was taken up by Prof. **Wilfred van Gunsteren**, professor emeritus and former Ombudsmann at ETH Zurich. He shared his thoughts and experiences regarding hiring, supervising as well as firing of doctoral students and postdoctoral fellows. As a common source for grievances he pointed out the size of a research group and recommended to choose it wisely in order to provide sufficient supervision to all group members. In the hiring process, cultural differences and expectations need to be taken into account, and the basis for judgment should involve a personal impression if possible. Prof. van Gunsteren recommended to be very clear with the expectations regarding the goal for doing a PhD or a postdoc, reporting, teaching and other infrastructural tasks, attendance of conferences and workshops, as well as the period and conditions of the employment. Furthermore, he gave advice how to keep group members motivated, which can be achieved for example by sufficient availability for discussions, adaptation of the supervising style to the needs and personality of the co-workers, clear distribution of group tasks, and organization of informal events. In the unhappy case that the cooperation with a PhD student or postdoc does not work out, it is important to decide it early and especially to be generous, such that there is sufficient time between the communication and the end of the employment. In the lively panel discussion that followed the two presentations, it was emphasized by both speakers that expectation management (in both directions) is a key element for the success or failure in supervision of co-workers.

After the coffee break, Prof. **Ulrich Aschauer** (University of Bern) presented the work of his group on oxynitrides using theoretical approaches. Oxynitrides with perovskite structure have attracted interest as catalysts to split water under visible light into hydrogen and oxygen. As mentioned in the morning by Dr. Emiliana Fabbri, hydrogen fuel is of high importance for renew-





able energy strategies. One obstacle that prevents current photocatalysts to reach higher efficiencies is charge-carrier recombination before the electron reaches the reactive surface sites. This effect could potentially be suppressed through surface charges created by the internal dipolar fields of polar materials. Prof. Aschauer explained how his group investigates the spontaneous polarization in strained oxynitride thin films *via* density functional theory (DFT) calculations. They could show that when the epitaxial

strain is sufficiently large, the anion order changes and the material becomes polar. This indicates that applying strain on oxynitride thin films could enhance the photocatalytic activity of these materials. Prof. Aschauer and his group are generally interested in water oxidation chemistry on transition metal oxides and the defect chemistry under external fields.

In the last talk of the meeting, Prof. **Laura Nyström** (ETH Zurich) introduced her group's investigations on the characterization of dietary fibres and methods to study health promotion. 38 million (*i.e.* 70%) deaths annually are caused by non-communicable diseases, while 80% of premature heart disease, stroke and diabetes could be prevented by a proper diet and abstaining from high-risk behaviors. Since fibre-rich foods promote good health by various means, like decreasing cholesterol and sugar



absorption in the gastrointestinal tract, Prof. Nyström's group studies the binding of small molecules to cereal β -glucans and oxidative modification in order to alter their health promoting and technological properties. She presented the Fenton-induced degradation of glucotetraoses, model compounds for β -glucan, *via* hydrophilic interaction UPLC-MS/MS. Her approach further involves selective enzymatic digestion, graphitized carbon solid phase extraction and functional group labeling. By combin-

ing such complementary sample preparation strategies, complete characterization of both lytic and non-lytic oxidation products is attainable. An important finding uncovered by her group is that the binding capacity of bile acids to β -glucans is not increased through oxidation, contrary to what was previously thought. In addition, her group used stopped flow spectroscopy to investigate Fenton reaction kinetics during β -glucan degradation in the presence of Fe^{2+} and concluded that iron binding is pH-dependent. As part of Prof. Nyström's ERC Starting Grant BINDING FIBRES, her objective is to understand non-covalent binding properties of dietary fibres with nutritionally relevant ligands.

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