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Chemistry
Platform of the Swiss Academy of Sciences

12th Young Faculty Meeting, 28th May 2019

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The Young Faculty Meeting (YFM) is an annual meeting of the young chemistry academics in Switzerland promoting scientific exchange and networking. It provides a rather unique opportunity for young group leaders at different stages of their careers to share the experience from their scientific independence with their peers. This year saw the 12th edition of the YFM to take place on May 28th in the Haus der Universität in Bern. It was organized by ***Tomáš Šolomek*** (Uni Basel), ***Pablo Rivera-Fuentes*** (ETH Zurich), and ***Leo Merz*** (SCNAT). The program consisted of six talks from outstanding young group leaders covering a rich variety of topics such as cellular signaling, solar energy conversion, machine learning, and others. Traditionally, these were complemented by three talks from senior guests on two hot topics in academia, the challenges and rewards of doctoral supervision, and the scientific outreach using social media platforms. The following informal but dynamic panel discussion of all attendees provided great incentives to think about the way we train the next generation of chemists and the advantages and pitfalls of social media in science.

Prof. Bill Morandi

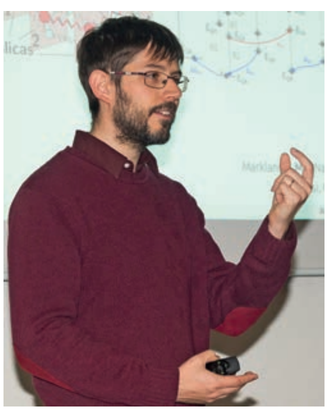
The program commenced by a round of introduction of all attendees and continued with ***Prof. Bill Morandi*** (ETH Zurich) introducing the concept of shuttle catalysis in organic synthesis for reversible functional group transfer. Inspired by the classical Meerwein-Ponndorf-Verley reduction and Oppenauer oxidation that both require the same catalyst, and are driven by the excess of one of the reagents, Morandi's group developed a series of useful transformations that allow to introduce, remove or exchange a functional group with the help of a homogeneous catalyst, even in a late stage of the synthesis. The first beautiful application showcased by Morandi involved transfer hydrocyanation between a nitrile and an alkene. No dangerous hydrogen cyanide needs to be used in this transformation, and the direction of the equilibrium can be controlled absolutely by the thermodynamic stability of the alkenes involved. He also demonstrated the possibility of a single bond metathesis, analogous to the well known alkene/alkyne metathesis. Here, carbon–sulfur and carbon–phosphorus bonds can be activated and a number of alkyl and aryl groups be exchanged. The trick to control the position of the equilibrium relies this time on the limited solubility of lithium alkylthiolate that is formed in the reaction as the by-product. The scope of the transformations is stunning, and it includes late-stage generation of a drug library, depolymerization of commercially available polyphenylenesulfide on gram-scale, or access to new phosphorus-based ligands and materials with fluorescent properties. The desire to understand the catalytic cycle led the group to isolate, crystallize, and characterize by X-ray diffraction the catalytic species involved in each step of the catalytic cycle. Each isolated organometallic complex naturally serves as the catalyst itself. Witnessing such interplay of synthetic methodology development with the help of the physical organic chemistry was truly pleasing for everyone in the audience. One of the current challenges that remain to be addressed is the activation of strong bonds, carbon-oxygen bonds in particular.

Prof. Sascha Hoogendoorn

Then the topic changed completely when ***Prof. Sascha Hoogendoorn*** (Uni Geneva) shared her passion for cellular signaling. In her research, she develops new molecular probes as chemical biology tools to provide an understanding of the underlying mechanisms with which cells communicate. One of her earlier achievements was the development of a synthetic mannose-6-phosphate (M6P) glycopeptide-based ligand to address mannose-6-phosphate receptors (MPRs). MPRs are ubiquitous on the surface of a variety of cell types, and, therefore, represent a promising class of receptors for targeted compound delivery into the endolysosomal compartments. She synthesized a conjugate of M6P-ligand, BODIPY fluorescent label, and DCG-04, an activity-based probe for cysteine cathepsins. Cathepsins belong to a family of proteases that mostly reside in the endolysosomal compartments. She showed that the M6PC–BODIPY–DCG-04 probe can label cathepsins in cells, and demonstrated its *in situ* uptake and trafficking. The Hedgehog (Hh) signaling pathway that is essential for embryonic development but also plays a role in cancer development, was discussed next. Enhancing or silencing this signaling pathway causes substantial developmental defects that Hoogendoorn supported with a very interesting story about cyclopamine, a teratogenic alkaloid found in corn lily that grows in the west of US. When fed to gravid sheep, lambs with a singular eye (cyclopia) were born, a consequence of interrupting the Hedgehog signaling pathway during fetus development. The molecular mechanisms of Hh signal transduction are, however, incompletely understood. For instance, many questions remain on the role of cilia, sensory organelles found on eukaryotic cells that orchestrate mammalian Hh signaling. "Can one identify all genes required for the cilium function?" asked Hoogendoorn the thought-provoking question. By developing a CRISPR/Cas9-based genetic screening platform, she indeed identified many hits important for signal transduction. In her own laboratory, established in the beginning of this year at the University of Geneva, she is now using a chemical biology approach which combines organic chemistry and genetic methodologies to further unravel ciliary signaling. Motivated students interested in this exciting topic should not hesitate and contact her because her lab is currently recruiting.

Prof. Victor Mougel

The next speaker was ***Prof. Victor Mougel*** (ETH Zurich) who strives to develop an electrolyzer with new catalysts for overall CO_2 reduction in neutral aqueous media to produce simple hydrocarbons. Cheap and effective CO_2 reduction with earth abundant catalysts represents the current scientific bottleneck for commercial deployment of this important process. The pH neutral conditions are important because H_2 formation dominates in highly acidic media, while CO_2 is converted at higher pH into bicarbonate and is no more available for reduction. One key issue was the absence of efficient electrocatalysts for water oxidation. His group has been developing high surface area dendritic copper/copper oxide materials as efficient catalysts for water oxidation. This was achieved by a nifty procedure when Cu is first electrodeposited at high current density. This resulted in intense formation of microbubbles of H_2 that acted as scaffold for the dendrite formation and a highly porous material. This material was further nanostructured by electrodeposition of CuO nanoparticles. Copper oxide has been used identified recently as a very promising precursor for CO_2 electroreduction catalyst. On that basis, the same dendritic copper/copper oxide material was used at both anode and cathode of an electrolyzer for CO_2 reduction. Another key factor that decreases the efficiency of CO_2 conversion is the mass transport of CO_2 to the surface of the cathode. To circumvent this issue, both electrodes were combined by Victor Mougel and coworkers in a continuous-flow electrochemical cell in which the anolyte and catholyte flow through the system. Constant saturation in CO_2 is ensured by continuously purging the catholyte with CO_2 in a separate compartment. Electroreduction of CO_2 in 0.1 M $CsHCO_3$ leads to structural changes at the cathode, the nanolayers of copper oxides being reduced to porous metallic copper containing voids resulting from nano-Kirkendall effect. The morphology of the resulting electrodes is stable even after prolonged electrolysis and shows remarkable selectivity for CO_2 reduction. This tailor-made electrolyzer for overall CO_2 reduction to hydrocarbons operates with a 21% energy efficiency, and with a benchmark 2.3% solar-to-hydrocarbon efficiency when coupled to perovskite photovoltaic cells.



Prof. Michele Ceriotti

After the coffee break, the meeting resumed with the talk of ***Prof. Michele Ceriotti*** (EPFL Lausanne) on machine learning. He explained the technicalities of machine learning approaches that are typically hidden to experimentalists behind complicated algorithms in a simplified and very engaging way. His group uses machine learning to predict, for example, the stability of different polymorphs of pharmaceuticals, or to compute NMR chemical shielding tensors of compounds in their solid state. The power of machine learning is in its speed and accuracy if the used train set to train the computer is sufficient. For instance, the solid NMR chemical shielding tensors can now be calculated with very good accuracy in only a fraction of time that a full density functional theory treatment would require. Identification of an outlier when the experimental and machine learning results are compared is relatively easy once the machine was sufficiently trained, and it provides great opportunity to test the available computational theories to understand such discrepant behavior. Ceriotti also demonstrated that the slopes of learning curves for a particular problem can be used to acquire useful information about the properties of the system. For example, an analysis of the slopes of the learning curves for models that are restricted to using information on short-range interparticle correlations reveals the characteristic length scale of interactions and how they affect the properties of the system. However, Michele Ceriotti kept probably the most important piece of information on machine learning to the conclusions where he relayed a story, due to Bertrand Russell, that summarizes the power and weakness of machine learning through the (mis)adventures of an inductivist turkey. If a turkey gets well fed every day of the week, on rainy and dry days, cold or warm, it concludes that each day brings the turkey another pleasure of a lavish meal. That is typically true until the Christmas comes, and the feast shifts onto a completely different table. In other words, the quality of a train set that one uses to train the computer is critical to the accuracy of the outcome and cannot get any better than the quality provided by the used train set.

The morning session was concluded by ***Dr. Oliver Renn*** (ETH Zurich) who is the head of the Information Center for Chemistry, Biology, and Pharmacy at ETH. His illuminative contribution on effective science communication by using Twitter as the platform for outreach could be considered one of the highlights of the program because it ignited a lively panel discussion in the afternoon. Oliver Renn commenced his talk with a poll to reveal that nearly 50% of the audience was convinced of the importance of Twitter for outreach, while the remaining half, divided into two equally populated groups, could not decide whether Twitter has more pros than cons, or thought that "there already is too much noise" in science communication, respectively. He then documented that since the birth of Twitter, it rapidly pervaded science, and became a considerable platform for science communication. A simple tweet using an account with a large number of followers impacts a large target audience when compared to the visibility of a scientific article on the publisher's webpage. Therefore, the outreach has transformed as a consequence of the birth of the social media platforms, both in terms of scholarly communication among peers and science communication to the public. Renn highlighted that Twitter is very important for young academics to make them stand out from the big crowd of other researchers. However, a scientist should do more than just tweet. A tweet contains 280 characters maximum, which is simply not enough to promote in-depth scientific discussion and explain the science to the public. Also, the number of active Twitter users among academics is steadily increasing. In the future, this may bring thousands of users to communicate science making the platform overwhelming to follow. Therefore, Renn promoted other software applications that allow scientists to communicate their work to laymen. Nevertheless, Twitter gets you noticed, increases the different visibility scores that help with your awareness through other channels, can help to make friends, and helps to serendipitously find important information. So do we really need to tweet our science? Well, the future will tell how science communication to our peers and the public gets transformed.

After lunch, the afternoon session continued with the science communication and inclusivity presented by ***Dr. Martina Ribar-Hestericová*** (Lonza), a forensic chemist, who is also a freelance

The discussions about the topics of the morning session continued during the lunch break.

science journalist maintaining a popular Instagram account dedicated to science outreach to the public. She focused not only on communicating the results of our scientific work to the world but also highlighted the importance of different channels that can deliver different outcomes useful to our own careers. For instance, Twitter brings visibility that can lead to enhancing the citation rate of our work but it is not the target platform that the younger generation follows. Should a scientist want to attract young students to the lab, Instagram can be a more suitable platform. She then addressed the typical fears that prevent people to join the social networks, such as fear of being wrong, ignored, yelled at, or simply the often unclear institutional rules that persist at universities. She also highlighted a study aimed at challenging the public stereotypes using selfies of scientists at their work. Interestingly, selfies of female scientist are perceived better by the public than those of their male colleagues, despite the generally observed gender inequality in science.

Prof. Athina Anastasaki

The talk of ***Prof. Athina Anastasaki*** (ETH Zurich) then returned to the domain of rigorous science. She introduced us to her research aimed at macromolecular chemistry. Her lab is interested in controlling the polymerization process initiated by radicals. For example, stereocontrol in cationic polymerization was successfully achieved a long time ago and allows to produce isotactic, syndiotactic, or atactic polymers or copolymers with high fidelity. However, such control is far from accomplished in radical polymerization because general conditions at which the polymerization would take place are difficult to find. Anastasaki clearly demonstrated that even a subtle change in the structure of a monomer can lead to polymers with very different properties in terms of molecular weight and dispersity, or even no polymerization at all. Therefore, optimizing the conditions to obtain the right polymer is one of the major challenges in the field. Her lab investigates atom transfer radical polymerization (ATPR) methods that may use light but typically a transition metal with two accessible oxidation states, for instance, copper, and external ligands to control the polymerization process. She surprised us by saying that polymerization can be achieved even with metallic copper and demonstrated such process by catalyzing a radical polymerization with an old British 2 pence coin. ATRP enables to polymerize a wide variety of monomers with different chemical functionalities that would normally be not tolerated in ionic polymerizations, and allows, therefore, to obtain heterostructures or different functional groups in the side-chains of the main polymer chain. Finally, the possibility of introducing automation into the field of radical polymerization was discussed.

Prof. Michael Saliba

The last scientific talk of the program was devoted to another hot topic in chemistry, hybrid organic–inorganic halide perovskite materials. ***Prof. Michael Saliba*** (University of Fribourg), undoubtedly one of the emerging stars in the field, shared a bit of history of perovskites and revealed the challenges the scientists must tackle to introduce the promising perovskite-based solar-energy conversion technologies onto the commercial markets. Perovskites are relatively easy to prepare using wet deposition techniques without the need for clean rooms. The color of the prepared material already unveils what phase resulted from the synthesis. The broad light absorption renders perovskites black, while the so-called yellow phase displays a very different crystal structure, and it lacks the desired properties of the black phase. The band gap of perovskites can be tuned by changing their chemical composition, *i.e.* by mixing different halides in various ratios, using different cations, or metal. The range of cations used in perovskites is limited by the tolerance factor for a cation in the perovskite crystal lattice. Too bulky cations lead to lattice distortions, and the ideal cation size ranges between ~1.6–2.6 Å. Saliba introduced the mixing of different cations in various ratios into the perovskite structure and demonstrated the positive effect of such composition. The introduction of Cs^+ leads to diminishing grain boundaries in the obtained material due to monolithic crystal growth. No post-synthetic annealing is required. The final material displays a promising photovoltaic effect with more than 20% power conversion efficiency and prolonged stability under visible light illumination. Only negligible changes could be observed after 200 h photovoltaic device performance. Michael Saliba then discussed the possibility of blending different metal ions into the perovskites instead of using a single metal, an approach that has been exclusively used in the past. Naturally, the mixing of different constituents introduces higher complexity and increases the chemical space that must be explored to discover the perfect perovskite material.

Prof. Antonio Togni (ETH Zurich) then delivered the last presentation of the day. He delved into a very important topic that gains increasing attention in academia, the rewards and challenges of doctoral (PhD) supervision. In view of the rate of dropout from graduate schools and recent reports on mental health issues of graduate students, discussion about good practices of supervision of PhD students is inevitable. Antonio Togni discussed real-life examples to demonstrate that PhD supervision is an important topic. For example, PhD students carry a significant share of research and teaching activities at strongly research-driven universities. In the past two decades, the number of PhD students in chemistry substantially increased, and the motivation for obtaining a doctorate for a majority is different from that observed more than 20 years ago. As a result, rethinking what the doctoral education actually is, consequently reshaping the curricula of graduate schools represents nowadays a necessity. Nevertheless, young academics that are becoming new principal investigators (PIs) do not typically receive any formal training regarding the supervision of students during their postdoc or graduate studies. Improving the leadership skills is therefore required to ease the increasing tension in a number of well-established labs, or to prevent such tension in those that are formed. ETH Zurich already organized the first Doctoral Supervision Symposium in January 2019 with more than 350 participants with a number of topics covered within the workshop, such as ethical aspects of supervision, communication culture within groups, bridging the gap between the PIs and PhDs, educating supervisors, or exchange of information on PhD supervision. The video footage from this symposium is available online.[1] How about rewards? One can say that there is more than new and original results, nice publications, high impact factors, and high reputation for and of the PI. Personal development of PhD students, both as scientists and independent thinkers is at least as important. Therefore, realizing that the support was worth the effort is a reward itself.

The day concluded with a dynamic panel discussion accompanied by an apéro where all participants freely interacted with the senior speakers Oliver Renn, Martina Ribar-Hestericová, and Antonio Togni. The hot topic of the day appeared to be the scientific outreach of scientists to their peers and the public that was debated in depth for over an hour and brought a number of new views and questions still to be answered in the future. The lively discussion at the end proved that the 12th Young Faculty Meeting 2019 in Bern was a success.

The lively final panel discussion with Dr. Martina Ribar Hestericová (left), Prof. Antonio Togni (middle) and Dr. Oliver Renn (right) about tweeting our science and doctoral supervision.

Received: July 16, 2019

[1] *https://www.video.ethz.ch/events/2019/supervision*