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Conference Report

Young Faculty Meeting 2024

AI in Chemistry: The Future of Discovery and Education?

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Certainly! I'd be happy to write a report on the Young Faculty Meeting 2024, based on the notes you provided. However, I have a few questions. Have you considered CHIMIA's submission guidelines? How will you check that the text is factual? And could you please ensure that your notes follow current standards on machine readable data structures?

Regular users of large-language models (LLMs), such as ChatGPT, may have already recognized that the above text was not machine-generated. Nevertheless, it neatly summarizes why this year's meeting of young chemistry professors in Switzerland – the Young Faculty Meeting 2024 (YFM2024) – chose the theme '*AI in Chemistry: The Future of Discovery and Education?*'. Since the release of ChatGPT3, the potential of artificial intelligence and machine learning (AI/ML) tools to transform the way we work and learn has caught the public's imagination and the associated technological innovations seem to progress at an astonishing pace. To assess and explore the potential impacts of AI/ML methods on research and education in Chemistry, YFM2024 invited experts, researchers, and practitioners to present the state-of-the-art in their fields, while offering the young faculty an opportunity to discuss their questions, concerns, and ideas.

For the first winter edition of the YFM, the SCNAT brought together about one-third of the chemical young faculty in Switzerland during a two-day meeting in February 2024 on Griesalp. Máté Bezdek, Rachel Hevey, Malte Oppermann, Patrick Steinegger and Leo Merz organized the meeting, which combined the topic of AI/ML in chemistry with talks from young faculty presenting their own research. Traditionally, the aim of the YFM is to connect young chemistry professors in Switzerland, to support their careers and to offer opportunities to learn and discuss about topics relevant to research, teaching and the scientific community. As in previous editions, the YFM2024 showcased the collaborative and welcoming spirit of the young chemistry faculty in Switzerland through insightful talks, lively conversations, and fun camaraderie. This year's program on AI/ML in chemistry was opened by ***Philippe Schwaller*** (EPFL), who gave an introductory lecture entitled 'Introduction to Machine Learning'. Covering the conceptual foundations of ML, he described its main approaches and highlighted that the associated training algorithms require high-quality data sets to achieve an efficient and reliable performance. Through examples, such as AlphaFold's tool to predict the three-dimensional structure of proteins from their amino acid sequence, the audience got a first glimpse of the potential scope of AI/ML tools in chemistry.

Following the opening lecture, ***Ross Milton*** (University of Geneva) pivoted the conference theme towards bioinorganic chemistry with his lecture entitled, 'Metalloenzyme (Electro)Catalysis for Hydrogen and Ammonia Production'. Seeking to understand the intricate molecular machinery behind the enzymes that activate some of the strongest bonds known in chemistry, Prof. Milton impressed upon the audience the power of mechanistic insight in designing new catalytic biotechnologies.

Maria Börner (Westernacher Solutions) then offered an application-focused perspective through her talk 'From AI Proof of Concept to Product', which explored current regulatory practices in the development of AI-based products. She confirmed that the quality and volume of the available data are key to achieving high product performances, hence data regulations, privacy concerns and copyright laws are central issues in the development of these products.

To bring the audience back to the world of chemistry, ***Murielle Delley*** (University of Basel) presented a lecture on 'Interfacial Chemistry and Catalysis of Inorganic Materials'. Through a case study on hydrogenation reactions catalyzed by cobalt phosphide, Prof. Delley demonstrated that fundamental thermochemical information about the strength of bonds formed at the surface of the metal catalyst can inform the outcomes of catalytic reactions. Additionally, Prof. Delley discussed her group's efforts to understand the nature of electrified interfaces using surface-enhanced IR spectro-electrochemistry (SIRS) with a look towards tunable catalysis.

Fig. 1. Panel discussion in front of the fireplace.

To conclude the afternoon programme, Philippe Schwaller, Maria Börner, and Michael Reutlinger (Roche) joined an interactive panel discussion (Fig. 1), moderated by Máté Bezdek and Malte Oppermann. Together with questions and comments from the audience, several topics related to AI/ML were discussed. For example, the use of LLMs for writing scientific publications emerged as a controversial topic, raising questions on authorship and copywriting, while also highlighting that writing up a scientific result can be seen as a tool that may simply be enhanced and accelerated with the help of AI-assistants. Further topics concerned the climate impact of AI/ML implementations, their impact on daily research practice and critical reflections on the limitations of current AI/ML tools.

Following a hearty dinner with lively conversations, the conference attendees re-convened for an evening session that began with a lecture by ***Patrick Steinegger*** (ETH Zurich/Paul Scherrer Institute) 'Following in the Footsteps of Mendeleev: Chemistry Experiments with Transactinide Elements'. In his lecture, Prof.

Steinegger illustrated how one can study elusive and extremely short-lived superheavy elements using the unique chemical and radiation 'fingerprints' they leave behind. Moreover, Prof. Steinegger made a logical and thought-provoking case for the feasibility (and importance) of keeping nuclear energy as part of the energy mix for a sustainable future.

As the final speaker of the first conference day, ***Jean-Rémy Marchand*** (Novartis) presented 'Computer-Aided Medicinal Chemistry in an Industrial Setting: Novartis'. Throughout this lecture, the audience was introduced to the considerations that industrial practitioners prioritize when using AI/ML tools to identify new chemical space in drug discovery. Dr. Marchand also articulated his firm belief that "*Machine learning/AI will not replace experimentalists, but experimentalists who use machine learning/AI will replace those who don't.*" Upon conclusion of the lecture, the day wrapped up on a light note, courtesy of ***Richard Smith*** (*Helvetica Chimica Acta*) and his hallmark Powerpoint Karaoke. In a laughter-filled session, conference attendees could showcase their impromptu presentation skills.

Against a spectacular Kiental backdrop (Fig. 2), the second day of the conference began with a workshop led by ***Andres Marulanda Bran*** (Schwaller Group, EPFL) entitled 'Practical AI Tools for Researchers'. Starting with literature search and management, he introduced *semanticscholar.org* and *perplexity.ai* and highlighted their context-based semantic search approaches. For code writing and data analysis, CodeLlama and ChatGPT were presented as powerful tools, whereas for image generation and processing a workflow involving several tools, such as Stable Diffusion and Clipdrop, were introduced, along with several practical examples.

Fig. 2. Group picture of the YFM 2024.

After a short coffee break, ***Alexandria Deliz Liang*** (University of Zurich) introduced her research group's activities in the areas of bioinorganic chemistry, protein and enzyme engineering. Specifically, Prof. Deliz Liang demonstrated how non-canonical amino acids can be used to alter enzymatic function with a case study on improving the reactivity of zinc-dependent hydrolytic enzymes.

Kjell Jörner (ETH Zurich) then presented how AI/ML tools are currently driving innovations in academic research in chemistry with a talk entitled 'Combining Machine Learning with Expert Knowledge'. He highlighted the interdisciplinary nature of the associated field of digital chemistry, which aims to improve the prediction of reaction outcomes, their optimization, and the design of chemical compounds. In addition, he explained how selecting the right combination of AI/ML model, training algorithm, data, and additional expert knowledge about the investigated chemical systems, can significantly improve the performance of the developed AI/ML tools.

Following the lunch break filled with stimulating discussions, the afternoon session began with the presentation of ***Nako Nakatsuka*** (EPFL) 'DNA-Gated Nanopores for Small-Molecule Biosensing'. In her talk, Prof. Nakatsuka presented her endeavors to understand fundamental molecular interactions both within DNA as well as between DNA and other small molecules. Prof. Nakatsuka described her aims to ultimately leverage this understanding for the design of better biosensing technologies, specifically to map chemical dynamics within the brain.

A complementary, industry-focused perspective was then provided by ***Michael Reutlinger*** (Roche) who introduced the application and scope of these tools in the discovery pipeline of the pharma sector through his talk titled 'ML/AI in small molecule research at Roche'. He particularly highlighted the key importance of high-quality data and how ML/AI tools can substantially improve the success rates in the identification of possible target compounds in the early stages of the discovery workflow.

The program on ML/AI was concluded through a presentation by ***Beatriz Borges*** (Bosselut Group, EPFL) entitled 'AI Assistants in Higher Education - Possibilities and Threats'. She described the advantages of LLMs and their text-generating capabilities as tools to enhance teaching, for example as interactive assistants, to generate practice problems and to accelerate administrative tasks, such as proof-reading and code writing. However, she also highlighted the current limitations and risks of these tools, such as the need to verify their output and their potential use for cheating in exams and assignments. Beatriz Borges then provided a succinct summary on the current state of AI/ML tools that equally holds for all areas covered at this year's YFM: AI/ML tools can be extremely useful and are here to stay, but to enhance their positive and minimize their negative impacts, they need to be carefully designed and trained on the right data.

As exemplified by the presentation excerpts above, over the course of two days, a broad array of ideas were exchanged amongst the YFM participants about the diverse settings in which AI/ML tools can be applied, and how best to apply them. Ultimately, all participants agreed that 'the jury is still out' on AI/ML, with only time being able to tell where their biggest impact will lie. However, it became very clear by the end of the conference that there is one thing that AI/ML tools cannot be, and that is, to be ignored.

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