

# Young Faculty Meeting 2024

## AI in chemistry: The future of discovery and education?

Location: Hotel Griesalp, Kiental, Switzerland

Organization: Máté Bezdek (ETH Zurich), Rachel Hevey (University of Basel), Malte Oppermann (University of Basel), Patrick Steinegger (ETH Zurich/Paul Scherrer Institute), Leo Merz (Swiss Academy of Sciences, SCNAT)

\*\*\* Thursday, February 1<sup>st</sup> 2024 \*\*\*

morning Arrival at Griesalp/[coffee](#)

10:45 **Round of introductions** (all participants)

12:10 **Murielle Delley** (University of Basel)  
*Interfacial Chemistry and Catalysis of Inorganic Materials*

12:30 [Lunch break](#)

14:00 **Philippe Schwaller** (EPFL / NCCR Catalysis)  
*Introduction to Machine Learning*

14:45 **Ross Milton** (University of Geneva)  
*Metalloenzyme (Electro)Catalysis for Hydrogen and Ammonia Production*

15:05 **Maria Börner** (Westernacher Solutions)  
*From AI Proof of Concept to Product*

15:50 [Coffee break](#)

16:30 **Jenn Chubb** (University of York) [online]  
*Speeding up to keep up? Implications of AI in the research process*

17:15 Interactive **panel discussion** with Philippe Schwaller, Maria Börner and Jenn Chubb

18:15 [Dinner break](#)

19:45 **Patrick Steinegger** (ETH Zürich / Paul Scherrer Institute)  
*Following in the Footsteps of Mendeleev: Chemistry Experiments with Transactinide Elements*

20:05 **Jean-Rémy Marchand** (Novartis)  
Computer-Aided Medicinal Chemistry in an Industrial Setting: Novartis

20:25 Powerpoint Karaoke with **Richard Smith** (Helvetica Chimica Acta)

\*\*\* Friday, February 2<sup>nd</sup> 2024 \*\*\*

- 08:30 **Andres Marulanda Bran** (LIAC-EPFL)  
*workshop: Practical AI Tools for Researchers*
- 10:00 *Coffee break*
- 10:30 **Alexandria Deliz Liang** (University of Zurich)  
*Genetic Code Expansion for Metalloenzyme Engineering*
- 11:10 **Kjell Jorner** (ETH Zurich)  
*Combining Machine Learning with Expert Knowledge*
- 11:55 *Lunch break*
- 14:00 **Nako Nakatsuka** (EPFL Neuro-X)  
*DNA-Gated Nanopores for Small-Molecule Biosensing*
- 14:20 **Michael Reutlinger** (Roche)  
*ML/AI in Small Molecule Research at Roche*
- 15:05 **Beatriz Borges** (EPFL)  
*AI Assistants in Higher Education - Possibilities and Threats*
- 15:50 **Malte Oppermann, Máté Bezdek**  
*closing remarks*
- 16:00 End/departure