Organizer: Prof. Dr. Frank Glorius glorius@uni-muenster.de
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University of Münster Corrensstraße 36
Institute of Organic Chemistry 48149 Münster

5TH INTERNATIONAL MINI-SYMPOSIUM

ON

MOLECULAR MACHINE LEARNING

JANUARY 19TH 2023 | 3:00 PM (UTC +1)

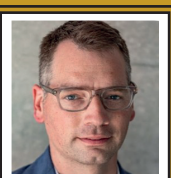
Núria López *Institut Català d'Investigació Química*, Spain
Kim Jelfs *Imperial College London*, UK
Tim Cernak *University of Michigan*, US
Sarah Reisman *California Institute of Technology*, US

Chair:
Frank Glorius *University of Münster*, Germany

SPEAKERS

Núria López graduated in Chemistry (1999) and got her Ph.D. degree in Theoretical Chemistry at the University of Barcelona, Spain (1995). As a postdoctoral researcher, she joined the Center for Atomic-scale Materials Physics led by Prof. Jens K. Nørskov (Denmark). In 2005 she started her independent career at ICIQ. Her research group focuses on the theoretical research in heterogeneous photo-electro-catalysis. Prof. López has also contributed to software development: Solvent contributions for VASP, Kinetic Monte-Carlo code, and the repository ioChem-BD, a computational catalysis database.

Dr. Kim Jelfs is a Professor in the Department of Chemistry at Imperial College London. Her group specialises in the use of computer simulations to assist in the discovery of supramolecular materials, particularly porous materials and organic electronics. Her research includes the development of open-source software to automate the assembly and testing of materials, with the application of artificial intelligence techniques including an evolutionary algorithm and machine learning. She carried out her PhD at University College London and a post-doc a the University of Liverpool.



Tim Cernak obtained a B.Sc. in Chemistry from UBC Okanagan studying the aroma profile of Chardonnay wines. Following a PhD in total synthesis with Prof. Jim Gleason at McGill University, Tim was a FQRNT Postdoctoral Fellow with Tristan Lambert at Columbia University. From 2009–2018, Tim worked with the Medicinal Chemistry team at Merck Sharp & Dohme in Rahway and Boston. Tim then joined the Department of Medicinal Chemistry at the University of Michigan in Ann Arbor as an Assistant Professor. The Cernak Lab is exploring an interface of chemical synthesis and data science. Tim is a co-Founder of Entos, Inc.

Professor Sarah Reisman earned a BA in Chemistry from Connecticut College in New London and her Ph.D. from Yale University, conducting research with Prof. John L. Wood in the area of total synthesis. As an NIH post-doctoral fellow, Sarah pursued studies in the field of asymmetric catalysis with Prof. Eric Jacobsen at Harvard University. In 2008, Sarah joined the California Institute of Technology where she is now the Bren Professor of Chemistry. Research in the Reisman lab seeks to advance chemical synthesis, through synergistic contributions in both strategy design for natural product synthesis and reaction development.

SCHEDULE: THURSDAY, JANUARY 19TH 2023

3:00 pm Introduction

3:10 pm **Núria López**
Machine Learning Tools in Heterogeneous Catalysis and Electrocatalysis
Activity, selectivity and stability are the key performance terms in catalysis by solids. Often, they can only be achieved with complex catalytic architectures where traditional Density Functional Theory can only model simple scenarios. Machine learning tools hold the key to circumvent many of the shortcomings of these models, and particularly can help merging experimental and computational simulations thus getting closer to a unified theory in catalysis.

3:40 pm **Kim Jelfs**
Remembering the Lab in Computational Molecular Materials Discovery
We have been developing computational software towards assisting in the discovery of molecular materials with targeted structures and properties. This includes the development of software to automate the assembly, structure and property prediction, including the use of an evolutionary algorithm to explore the possible phase space, and machine learning to accelerate predictions. We work closely with experimental collaborators and so considering the synthesis of the materials is central to our approach, including a recently development machine learning model that predicts a chemist's opinion on the ease of synthesis of the material.

4:10 pm Break

4:30 pm **Tim Cernak**
Information Rich Retrosynthesis Tactics
The chemical synthesis of molecules gives society so many of the products we enjoy daily like medicines, agrochemicals, and plastics. While nearly any molecule can in principle be synthesized, devising practical synthetic routes remains a significant challenge. In fact, the design of chemical products is heavily influenced by how easily the products can be synthesized. This presentation will discuss new strategies and tactics for identifying efficient retrosynthetic routes, often leveraging reactions that still need to be invented.

5:00 pm **Sarah Reisman**
The Development and Application of Data-Driven Tools for Synthetic Organic Chemistry
Artificial intelligence (AI) has modernized the scientific method, bringing predictive power to fields in a broad range of disciplines. Organic chemistry has been relatively slow to adopt machine learning (ML) methods, although recently there has been growing interest in developing predictive models that accelerate reaction discovery. These methods provide new tools to help chemists predict reaction yields or identify suitable reaction conditions. This lecture will focus on our efforts to develop and apply new ML methods for reaction condition prediction and reaction optimization tasks.

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SPP 2363

Starting Times	
Beijing	9:00 pm
New Delhi	6:30 pm
Paris	3:00 pm
London	2:00 pm
New York	9:00 am

Please find the registration and
Zoom invitation using the following link:
www.uni-muenster.de/Chemie.oc/glorius/symposium_mml.html