Organizer: Prof. Dr. Frank Glorius glorius@uni-muenster.de
Co-Organizer: Florian Boser florian.boser.ml@uni-muenster.de
University of Münster Corrensstraße 36
Institute of Organic Chemistry 48149 Münster

7TH INTERNATIONAL MINI-SYMPOSIUM

ON

MOLECULAR MACHINE LEARNING

JANUARY 16TH 2025 | 3:00 PM (UTC +1)

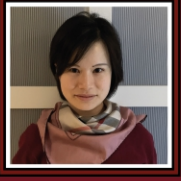
Heather J. Kulik *Massachusetts Institute of Technology*, USA
Fernanda Duarte *University of Oxford*, UK
Bingqing Cheng *University of California, Berkeley*, USA
Matthew S. Sigman *University of Utah*, USA

Chair:
Frank Glorius *University of Münster*, Germany

SPEAKERS

Heather J. Kulik is the Lammot du Pont (1901) professor in the Departments of Chemical Engineering and Chemistry at MIT. She received her B.E. in Chemical Engineering from the Cooper Union in 2004 and her Ph.D. from the Department of Materials Science and Engineering at MIT in 2009. She completed postdoctoral training at Lawrence Livermore and Stanford, prior to joining MIT as a faculty member in 2013. Her research has been recognized by a DARPA Young Faculty Award and Director's, Sloan and Hans Fischer Fellowship, NSF CAREER Award, among others.

Fernanda Duarte obtained her PhD from Pontificia Universidad Católica de Chile. As a postdoctoral researcher she trained in biomolecular modelling with Prof. Lynn Kamerlin at Uppsala University and in computational organic chemistry with Prof. Robert Paton at the University of Oxford as a Newton Fellow. After a brief period as a lecturer at the University of Edinburgh she returned to Oxford in 2018 as an Associate Professor. Her research combines computational developments with practical applications spanning multiple systems' sizes, from enzymes to small molecules.



Bingqing Cheng is an Assistant Professor at UC Berkeley. Prior to that, she was an Assistant Professor at IST Austria. She obtained her PhD in Materials Science from EPFL in 2019. After graduation, she became a Junior Research Fellow at Trinity College, University of Cambridge, and then in 2020, a Departmental Early Career Fellow in the Department of Computer Science and Technology in Cambridge. She has won the Volker Heine Young Investigator Award, JCP Best Paper by an Emerging Investigator Award, and the ERC starting grant.

Matt Sigman is Distinguished Professor at the University of Utah. He received a B.S. in chemistry from Sonoma State University in 1992 before obtaining his Ph.D. at Washington State University with Professor Bruce Eaton in 1996 in organometallic chemistry. He then moved to Harvard University to complete a postdoctoral stint with Professor Eric Jacobsen. In 1999, he joined the faculty of the University of Utah where his research group has focused on the development of new synthetic methodology with an underlying interest in reaction mechanism.

SCHEDULE: THURSDAY, JANUARY 16TH 2025

3:00 pm Introduction

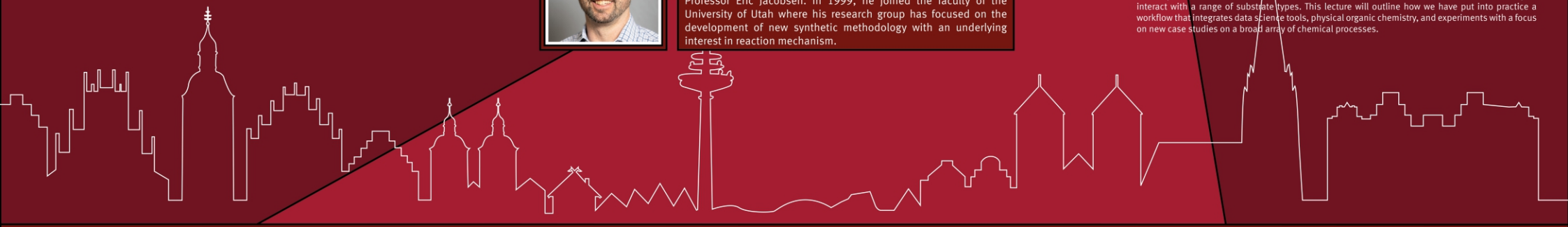
3:10 pm **Heather J. Kulik**
Getting from the Computer to Real World Materials Faster with Machine Learning
I will discuss our efforts to accelerate the discovery of novel transition metal-containing materials using machine learning. This includes leveraging experimental datasets through text mining and semantic embedding to uncover relationships between structure and function. I will then highlight how we utilized large datasets of synthesized materials to uncover those with novel function in polymer networks. The success of our design strategy will be demonstrated through macroscopically visible changes in network scale properties.

3:40 pm **Fernanda Duarte**
Modelling Chemical Reactions in Solution with Machine Learning Potentials – Balancing Efficiency and Accuracy
While computational characterisation of reaction energy pathways has become routine, accurately accounting for solvent and dynamic effects remains a significant challenge. Machine learning potentials (MLPs) offer a promising alternative to traditional ab initio methods by enabling high efficiency and accuracy. This talk introduces efficient strategies for training reactive MLPs with minimal computational cost. Enhanced sampling techniques are employed to train MLPs where little knowledge of the PES is available. We examine the impact of descriptors, model architectures, training methodologies, and evaluation metrics on the performance and accuracy of MLPs.

4:10 pm Break

4:30 pm **Bingqing Cheng**
Predicting Material Properties with the Help of Machine Learning
A central goal of computational chemistry is to predict material properties using first-principles methods based on the fundamental laws of quantum mechanics. However, the high computational costs of these methods typically prevent rigorous predictions of macroscopic quantities at finite temperatures. I will demonstrate how to enable such predictions by combining advanced statistical mechanics with machine learning interatomic potentials. I will show example applications on computing the phase diagrams, chemical potentials of mixtures, adsorption isotherms of gas in porous materials, and reactions on surfaces.

5:00 pm **Matthew S. Sigman**
Developing Data Science Tools for Synthetic Chemists
We developed several data science and machine learning tools that assist in designing the proper experiments to facilitate the analysis of structure function relationships while also providing platforms for reaction optimization. Specifically, we have used new methods to develop descriptors for complex molecular architectures as well as data science methods to discern how these catalysts interact with a range of substrate types. This lecture will outline how we have put into practice a workflow that integrates data science tools, physical organic chemistry, and experiments with a focus on new case studies on a broad array of chemical processes.



Universität Münster

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:
https://bit.ly/7thMML