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University of Münster Corrensstraße 36
Institute of Organic Chemistry 48149 Münster

4TH INTERNATIONAL MINI-SYMPOSIUM

ON

MOLECULAR MACHINE LEARNING

JANUARY 13TH 2022 | 3:00 PM (UTC +1)

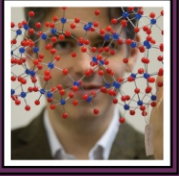
Bartosz A. Grzybowski *UNIST*, South Korea; *PAN*, Poland
Anat Milo *Ben-Gurion University*, Israel
Lee Cronin *University of Glasgow*, UK
Karsten Reuter *Fritz-Haber-Institut*, Germany

Chair:
Frank Glorius *University of Münster*, Germany

SPEAKERS

Bartosz A. Grzybowski is a Distinguished Professor of Chemistry at the IBS Center for Soft and Living Matter and Professor at the Polish Academy of Sciences. Although he has spent a large fraction of his research on esoteric problems of self-assembly and non-equilibrium systems, he considers his most impactful discoveries to be in the area of computer-driven synthesis. Grzybowski started several companies with capitalization close to $1 billion, and has advised industrial and governmental bodies in areas from AI to oil drilling.

Anat Milo studied chemistry at the Hebrew University of Jerusalem and UPMC Paris before obtaining her Ph.D. from the Weizmann Institute of Science with Ronny Neumann. After her postdoctoral studies at the University of Utah with Matthew Sigman she returned to Israel at the end of 2015 to join the Department of Chemistry at Ben-Gurion University of the Negev, where her research group develops experimental, statistical, and computational strategies for identifying molecular design principles in catalysis.



Leroy (Lee) Cronin is the Regius Professor of Chemistry in Glasgow. His research spans many disciplines and has four main aims: the construction of artificial life; the digitization of chemistry; the use of artificial intelligence in chemistry and the construction of 'wet' chemical computers; the exploration of complexity and information in chemistry. His group is assembled transparently around ideas, avoids hierarchy, and aims to mentor researchers using a problem-based approach. Nothing is impossible until it is tried.

Karsten Reuter is Director of the Theory Department at the Fritz Haber Institute (FHI) of the Max Planck Society in Berlin. He obtained his Ph.D. in theoretical physics from Universität Erlangen–Nürnberg in 1998. Following various positions at the FHI and the FOM Institute for Atomic and Molecular Physics in Amsterdam, he was Full Professor for Theoretical Chemistry at the Technical University of Munich from 2009 to 2020 until he returned to the FHI in his current position.

SCHEDULE: THURSDAY, JANUARY 13TH 2022

3:00 pm Introduction

3:10 pm **Bartosz A. Grzybowski**
Synthesis in the age of computers: From synthesis planning to reaction discovery
After decades of somewhat unsuccessful attempts, computers are finally making impact on the practice of synthetic chemistry. This change is made possible by the combination of increased computing power and, above all, new algorithms to encode and manipulate synthetic knowledge at various levels, from sequences of full reactions to sequences of mechanistic steps. In my talk, I will illustrate how these advances have enabled completely autonomous planning of multistep syntheses of complex (natural product) targets, and how they allow us to discover new methodologies and unprecedented reaction types.

3:40 pm **Anat Milo**
Statistics are a girl's best friend: Expanding the mechanistic study toolbox with data science
The value of amassing and standardizing chemical Big Data for improving the efficiency of chemical discovery is becoming increasingly clear. However, in many cases, we do not have the means to produce large data sets, so by necessity we remain in the Small Data regime. In this talk, I will present our work in the field of organocatalysis focused on applying machine learning strategies to small data sets as a means to uncover underlying mechanisms. We aim to show that exploring Small Data is not just a necessity, but can be key to bridging the gap between human intuition and machine learning.

4:10 pm Break

4:30 pm **Lee Cronin**
Chemputation
I will outline how we have devised a universal approach to chemical synthesis and discovery using the process of chemputation – a robotic system, driven by chemical intelligence algorithms, designed to search for new reactivity, reactions, and molecules. To achieve this, we have built a programmable robotic discovery system that can run the reactions and analysis. To program the robot, we exploit the world's first domain-specific chemical programming language (XDL) to produce the code. This system will handle the programming of robots so expert chemists can focus on generating discovery experiments, allowing the exploration of chemical space.

5:00 pm **Karsten Reuter**
From Computational Discovery toward Data-Driven Design of Molecules and Materials
The vastness of chemical spaces dictates search strategies for functional molecules and materials beyond the manual and intellectual throughput of human investigators. Efforts like descriptor engineering or machine-learning (ML) surrogate models for demanding first-principles calculations aim to increase the throughput by generating larger databases for computational screening. In this talk I will discuss our efforts to complement this with advanced search strategies like active learning that query the data on demand. Apart from an increased data efficiency, this represents first steps from a mere discovery towards true data-driven design.

WWU MÜNSTER

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