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 exotter problems of self-assembly and non-equilibrium systems, he considers his most important 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 UPMPD 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.

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 next-generation 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 1996, 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 incremental computational 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 outline how these advances have enabled continuous autonomous planning of multistep synthesis of complex (e.g., product) targets, and how they allow us to discover new methodologies and unexpected 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 analyzing 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 as necessary moves towards the Small Data regimen. In this talk, I will present in depths of a data anthropologist’s toolkit some small data based data science tools used to unravel underlying mechanisms. We aim to show that exploring Small Data is not just necessary, but can be key to bridging the gap between human intuition and machine learning.

4:10 pm Break

4:30 pm Lee Cronin
Chemputer

I will discuss how we have devised a universal approach to chemical synthesis and discovery using the process of chemoprinting—a robotic system, driven by chemical intelligence algorithms, designed to search for new materials, reactions, and mechanisms. To achieve this, we have built a programmable robotic discovery system that can run the machines and analyze. I will present the results of our first discovery tests, and some initial scientific programming language (SPLP) to improve the code. This system will further the programming of syntheses so expert chemists can focus on interpreting 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 field of chemical computing involves search strategies for functional molecules and materials toward the design and optimization of new materials. Hence, the development of machine learning (ML) on such problems for designing molecules and materials. In this talk, I will outline our efforts to complement ML-based search strategies with new architectural strategies to accelerate the search. Machine learning algorithms can be used to accelerate the search for improved molecule databases for computational screening. In this talk, I will present our efforts to complement ML-based search strategies with new architectural strategies to accelerate the search for improved molecule databases.