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Co-Organizer: Philipp Pflüger p_pflu02@uni-muenster.de
University of Münster Correnstraße 40
Institute of Organic Chemistry 48149 Münster

International Mini-Symposium

on

Molecular Machine Learning

July 9th 2020 **3:00 pm (UTC +2)**

Regina Barzilay Massachusetts Institute of Technology, USA
Anatole von Lilienfeld University of Basel, Switzerland
Jürgen Bajorath University of Bonn, Germany
Philippe Schwaller IBM, Switzerland

Chair:
Frank Glorius University of Münster, Germany

Speaker

Regina Barzilay is a professor in the Department of Electrical Engineering and Computer Science and a member of the Computer Science and Artificial Intelligence Laboratory at the MIT. Her research interests are in natural language processing. Currently, Prof. Barzilay is focused on bringing the power of machine learning to oncology. Prof. Barzilay is poised to play a leading role in creating new models that advance the capacity of computers to harness the power of human language data.

As of this fall, Anatole von Lilienfeld will join the Faculty of Physics at the University of Vienna as a professor of Computational Materials Discovery. Currently, he is an associate professor of Physical Chemistry at the Department of Chemistry of the University of Basel. In 2016, he was an associate professor at the University of Brussels after having spent two years as a Swiss National Science Foundation professor at the University of Basel prior to which he worked for Argonne and Sandia National Laboratories.

Jürgen Bajorath is Professor and Chair of Life Science Informatics at the University of Bonn. For the past decade, his research has mostly focused on the development of computational methods for medicinal chemistry. Among others, current research topics include large-scale analysis and visualization of structure-activity relationships, exploration and prediction of multi-target activities of small molecules, big data concepts, and data-driven design of novel active compounds.

Philippe Schwaller is currently a PhD student in the Reymond Group at the University of Bern and a predoctoral researcher at IBM Research in Zurich. He received a bachelor's and master's degree in Materials Science and Engineering from EPFL and an MPhil degree in Physics from the University of Cambridge. Since he joined IBM Research in March 2017, his main focus is on machine learning for accelerating the discovery and synthesis of novel molecules and materials.

Schedule: Thursday July 9th, 2020

3:00 pm Introduction

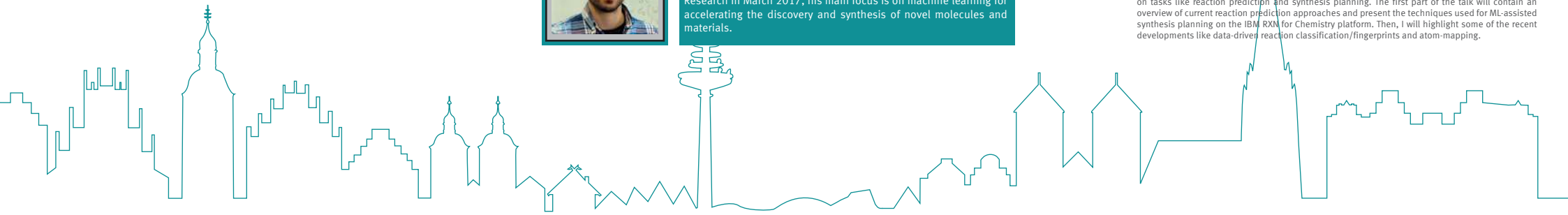
3:05 pm **Regina Barzilay**
Learning Molecular Representation
State-of-the-art approaches for learning molecular representations are based on graph convolutional neural networks. While these representations are shown useful for property prediction and molecular generation, they have a number of deficiencies that limit their ability to capture important molecular properties. In this talk, I will summarize our recent work aiming to improve generalization capacity and expressiveness of these models

3:35 pm **Anatole von Lilienfeld**
Quantum Machine Learning
Many of the most relevant observables of matter depend explicitly on atomistic and electronic details, rendering a first principles approach to computational materials design mandatory .Alas, even when using high-performance computers, brute force high-throughput screening of material candidates is beyond any capacity for all but the simplest systems and properties due to the combinatorial nature of compound space, i.e. all the possible combinations of compositional and structural degrees of freedom. Consequently, efficient exploration algorithms exploit implicit redundancies and correlations. I will discuss recently developed statistical learning based approaches for interpolating quantum mechanical observables throughout compound space. Numerical results indicate promising performance in terms of efficiency, accuracy, scalability and transferability.

4:05 pm Break

4:15 pm **Jürgen Bajorath**
Compound Activity Predictions at Different Levels of Complexity
Machine learning has been a mainstay in chemoinformatics for nearly 20 years, with a variety of applications in compound classification and property prediction. Recently hyped compound design strategies employing deep learning architectures only represent a part of the spectrum. While fundamental challenges for machine learning in pharmaceutical research have remained essentially unchanged over the years, there are many opportunities going forward. Exemplary applications are presented that illustrate the utility and limitations of machine learning in different compound prediction and design scenarios.

4:45 pm **Philippe Schwaller**
Learning the Language of Chemical Reactions Using Transformer Based Models
Artificial intelligence is currently revolutionising chemical research. Particularly in automated synthesis, modern natural language processing technologies have achieved unprecedented results on tasks like reaction prediction and synthesis planning. The first part of the talk will contain an overview of current reaction prediction approaches and present the techniques used for ML-assisted synthesis planning on the IBM RXN for Chemistry platform. Then, I will highlight some of the recent developments like data-driven reaction classification/fingerprints and atom-mapping.



WWU MÜNSTER

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

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