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University of Münster Correnstraße 40
Institute of Organic Chemistry 48149 Münster

2ND INTERNATIONAL MINI-SYMPOSIUM

ON

MOLECULAR MACHINE LEARNING

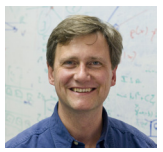
JANUARY 14TH 2021 | 3:00 PM (UTC +1)

Abigail Doyle Princeton University, USA
Klaus-Robert Müller Technical University of Berlin, Germany
Alán Aspuru-Guzik University of Toronto, Canada
Connor Coley Massachusetts Institute of Technology, USA

Chair:
Frank Glorius University of Münster, Germany

SPEAKERS

Abigail Doyle is the A. Barton Hepburn Professor of Chemistry in the Chemistry Department at Princeton University. She obtained her Ph.D. in catalysis and physical organic chemistry at Harvard University in 2008 under the direction of Prof. Eric Jacobsen after receiving her A.B. and A.M. in chemistry and chemical biology from Harvard in 2002. She joined at Princeton University in 2008 and is currently a co-PI for the NSF CCI Center for Computer Assisted Synthesis and the DOE EFRC Bioinspired Light-Escalated Chemistry.



Klaus-Robert Müller (Ph.D. 92) has been a Professor of computer science at TU Berlin since 2006 and is the director of Berlin Institute for the Foundations of Learning and Data. For three decades he has enjoyed contributing to basic research in Machine Learning and his special focus is on Machine Learning in the sciences: neurosciences, cancer research and most recently quantum chemistry. He is an elected member of the German National Academy of Sciences Leopoldina and ISI highly cited researcher.

Alán Aspuru-Guzik's research lies at the interface of computer science with chemistry and physics. He works in the integration of robotics, machine learning and high-throughput quantum chemistry for the development of materials acceleration platforms. He is jointly appointed as a Professor of Chemistry and Computer Science at the University of Toronto. Alán is a faculty member of the Vector Institute for Artificial Intelligence. Previously, Alán was a full professor at Harvard University where he started his career in 2006.

Connor W. Coley is an Assistant Professor at MIT in the Department of Chemical Engineering. His work in computer assistance and automation for organic synthesis has included the development of a data-driven synthesis planning program and in silico strategies for predicting the outcomes of organic reactions. His continuing research interests are in how data science, statistical learning, and laboratory automation can be used to streamline discovery in the chemical sciences.

SCHEDULE: THURSDAY, JANUARY 14TH 2021

3:00 pm Introduction

3:10 pm **Abigail Doyle**
Machine Learning for Experimental Synthetic Chemists
Numerous disciplines, such as image recognition and machine translation, have been revolutionized by using machine learning (ML) to leverage big data. In organic synthesis, providing accurate chemical reactivity prediction with ML models could assist chemists with reaction prediction, optimization, and mechanistic interrogation. This talk will cover my group's efforts on experimental data collection and the quest to expand its availability and limit its bias for data science application; feature engineering that may extend common intuition about the underlying chemistry; model assessments in the regime of small to medium size reaction datasets; and opportunities arising from accurate model predictions and their mechanistic interpretation.

3:40 pm **Klaus-Robert Müller**
Machine Learning for the Sciences - Towards Understanding
This talk will discuss recent developments of Machine Learning techniques for quantum chemistry. One focus will be the usage of explainable AI techniques to obtain novel insights for the sciences from machine learning models.

4:10 pm Break

4:30 pm **Alán Aspuru-Guzik**
There is no Time for Science as Usual: Materials Acceleration Platforms
The world is facing several time-sensitive issues ranging from climate change to the rapid degradation of our climate, as well as the emergence of new diseases like COVID-19. We need to rethink the way we do science and think of it as a workflow that could be optimized. Where are the pain points that can be solved with automation, artificial intelligence, or better human practices? My group has been thinking about this question with an application to the design of organic optoelectronic materials. In this talk, I will discuss the progress in developing materials acceleration platforms, or self-driving labs for this purpose.

5:00 pm **Connor Coley**
Data-Driven Chemical Synthesis
This talk will describe ongoing efforts to streamline the design, validation, and implementation of small molecule synthetic routes through a computational understanding of synthetic chemistry learned from the chemical literature. We have developed an open source software suite, ASKCOS, that is capable of proposing retrosynthetic routes to new molecules, proposing reaction conditions for each step, and assessing the likelihood of experimental success. A proof-of-concept demonstration shows how these tools, in combination with laboratory automation and robotics, can streamline chemical development.

WWU MÜNSTER

Starting Times	
Beijing	10:00 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 following link:
www.uni-muenster.de/Chemie.oc/glorius/symposium_mml.html