



Machine Learning Hits the Lab: Experiment Planning with Bayesian (Co-)Pilots

Prof. Dr. Felix Strieth-Kalthoff
Juniorprofessor für Digitale Chemie,
Bergische Universität Wuppertal,
Fakultät für Mathematik und
Naturwissenschaften,
Gaußstraße 20,
42119 Wuppertal

18. November 2024
16:00 Uhr
Hörsaal FZH3
Campus Freudenberg

www.cmats.uni-wuppertal.de

■ Chemistry and materials science regularly involve decision-making tasks of varying complexity, ranging from selecting which material to synthesize and test, over choosing reaction conditions, to setting instrument parameters. These problems are often high-dimensional and nonlinear, suggesting they could benefit from machine learning (ML).

■ In this talk, I will discuss some of our recent efforts to integrate Bayesian ML tools into experimental laboratory workflows. A particular focus will be on addressing data limitations by enhancing ML with expert knowledge to improve decision making. Using examples from synthetic chemistry and conjugated organic materials discovery, the talk will highlight the opportunities and challenges in ML to support lab-based decisions.