JCF-Vortrag am 07.05.26

17:15 Uhr, OC-Hörsaal

Prof. Dr. Felix Strieth-Kalthoff
Digital Chemistry
(Universität Wuppertal)

Towards Practical Experiment Planning with Machine Learning
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Award for the Best Bachelor's and Master's Theses

Chemistry and materials science regularly involve decision-making tasks of varying complexity – from selecting which material to synthesize and test, to choosing reaction conditions, to configuring instrument parameters. These problems are often high-dimensional and nonlinear, suggesting they could be addressed using machine learning (ML). Over the last decade, Bayesian ML has been widely established for effective decision making under uncertainty, and has gained traction in chemistry in recent years. In this talk, I will discuss some of our recent efforts to incorporate Bayesian ML tools into experimental workflows. Using case studies from synthetic chemistry and functional molecule discovery, the talk will highlight the opportunities and challenges in ML to support laboratory decision making.

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