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Machine Learning for Accelerated Molecular Discovery

Monday, 19 September 2022 16:30 (45 minutes)

Machine learning can enable and accelerate the design of new molecules and materials in multiple ways, e.g. by learning from large amounts of (simulated or experimental) data to predict molecular or materials properties faster, or even by interfacing machine learning algorithms for autonomous decision-making directly with automated high-throughput experiments. This talk will give a brief overview of our research activities on graph neural networks for materials property prediction [1], machine learning accelerated atomistic simulations of photochemical reactions [2,3], as well as on the machine learning based prediction of synthesis conditions for metal-organic frameworks [4].

[1] Reiser et al., Software Impacts 2021, https://www.sciencedirect.com/science/article/pii/S266596382100035X
[2] Friederich et al., Nature Materials 2021, https://www.nature.com/articles/s41563-020-0777-6
[3] Li et al., Chemical Science 2021, https://pubs.rsc.org/en/content/articlehtml/2021/sc/d0sc05610c
[4] Luo et al., Angewandte Chemie 2022, https://onlinelibrary.wiley.com/doi/full/10.1002/anie.202200242

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