

Machine Learning for Design and Autonomous Discovery of Materials and Molecules

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Machine learning can accelerate the screening, design, and discovery of new molecules and materials in multiple ways, e.g. by virtually predicting properties of molecules and materials, by extracting hidden relations from large amounts of simulated or experimental data, or even by interfacing machine learning algorithms for autonomous decision-making directly with automated high-throughput experiments. In this talk, I will focus on our research activities on graph neural networks for property prediction [1] and inverse design of crystal structures using Bayesian flow networks [2], as well as on the use of active learning in self-driving labs, especially in the area of organic semiconductors for photovoltaics [3,4].

Reference:

- [1] Reiser et al., Communications Materials 3, 93 (2022), <https://www.nature.com/articles/s43246-022-00315-6>
- [2] Under review in ICML 2025
- [3] Wu et al., JACS 145, 30, 16517–16525 (2023), <https://pubs.acs.org/doi/full/10.1021/jacs.3c03271>
- [4] Wu et al., Science 386, 6727, 1256-1264024 (2024),
<https://www.science.org/doi/abs/10.1126/science.ads0901>

Bio

After his B.S. and M.Sc. in physics and a Ph.D. in physics on multiscale modeling of organic semiconductors, Pascal Friederich received a Marie-Sklodowska-Curie Postdoctoral Fellowship at Harvard University and the University of Toronto where he worked on machine learning methods for chemistry. In 2020, Pascal Friederich joined the Informatics Department of the Karlsruhe Institute of Technology as a tenure-track professor, leading the AI for Materials Science (AiMat, <https://aimat.science>) research group. The AiMat research group focuses on developing and applying machine learning methods for property prediction, simulation, understanding, and design of molecules and materials, as well as on interfacing machine learning methods with automated materials experiments. In 2022, Pascal Friederich received the Heinz-Maier-Leibnitz Prize from the German Research Foundation.