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Active learning for accelerated discovery and materials optimisation

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Time: **Tuesday, June 18, 2024, 8:50**

Location: **Lise Meitner Lecture Hall**
9. Boltzmanngasse 5

Data-driven materials science based on artificial intelligence (AI) methods has facilitated breakthroughs in materials optimization and design. Of particular interest are active learning algorithms, where datasets are collected on-the-fly in the search for optimal solutions. We encoded such a probabilistic algorithm into the Bayesian Optimization Structure Search (BOSS) tool for materials optimization [1]. This versatile approach was utilised to study molecular surface adsorbates [2], thin film growth [3], solid-solid interfaces [4], molecular conformers [5] and even optimise experimental outcomes [6]. The smart sampling strategy allows to infer optimal solutions with modest datasets, saving time and resources. Further algorithm developments will allow us to harness multiple channels of information and further accelerate the development of materials for next-generation technologies.

[1] npj Comput. Mater., 5, 35 (2019)
[2] Beilstein J. Nanotechnol. 11, 1577-1589 (2020), Adv. Func. Mater., 31, 2010853 (2021)
[3] Adv. Sci. 7, 2000992 (2020)
[4] ACS Appl. Mater. Interfaces 14 (10), 12758-12765 (2022)
[5] J. Chem. Theory Comput. 17, 1955 (2020)
[6] MRS Bulletin 47, 29-37 (2022)

As part of the presentation, there will be a teaching demonstration on the topic "Einstein and Debey Model".