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Vienna Doctoral School in Physics

ESI Erwin Schrödinger International Institute for Mathematics and Physics

Machine Learning for Materials Hard and Soft

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Computational materials engineering with active learning

Abstract:
Data-driven materials science based on artificial intelligence algorithms has facilitated breakthroughs in materials optimization and design. Of particular interest are active learning techniques, where datasets are collected by sampling on-the-fly in the search for optimal solutions. We encoded such a probabilistic algorithm into the Bayesian Optimization Structure Search (BOSS) Python tool for materials research. We applied this versatile tool to study functional materials, like molecular surface adsorbates, thin films, solid-solid interfaces, molecular conformers, and even to optimise experimental outcomes. Agreement between optimal solutions and experimental measurements suggests that active learning is capable of good accuracy at computational costs up to 10 times smaller than other approaches. New algorithms combining batch and gradient acquisitions with multi-fidelity schemes will allow us to harness the power of exascale computing platforms for next-generation materials engineering.

FWF Der Wissenschaftsfonds.
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