

## **Efficient Materials Discovery Enabled by AI-Guided Workflows and Accurate Non-Local Density Functional Theory Calculations**

AI-guided workflows will accelerate the discovery of new materials. In particular, AI can be used in conjunction with a data-acquisition strategy in order to iteratively identify materials that present the desired properties, out of immense pools of uninteresting candidates. However, the efficiency of AI approaches currently applied in iterative materials-discovery strategies often relies on the knowledge of few, key input parameters or features required to describe a certain materials property. This is a drawback in materials science because these key parameters are typically unknown. Besides, high-quality datasets are often small. Here, we develop an AI-guided workflow based on the sureindependence-screening-and-sparsifying-operator (SISSO) approach. By using moderate amounts of data, the SISSO symbolic-regression approach identifies models of material properties as analytical expressions depending on key physical parameters, out of many initially offered ones. Crucially, we train ensembles of SISSO models and obtain mean predictions and prediction uncertainties. We analyze the quality of uncertainty estimates and their suitability to steer the acquisition of data in unseen portions of materials space. The SISSO-guided workflow is applied to identify acid-stable oxides for electrocatalysis based on DFT-HSE06 calculations.