Unlocking Materials Discovery: AI-Driven Workflows

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

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In Short

- Stable oxides
- Multi-fidelity modelling
- Workflow

Materials are integral to diverse sectors, including renewable energy, manufacturing, transportation, and information technology. They are crucial for the development of photovoltaic devices, catalytic reactions, and other applications. However, existing materials face challenges in terms of efficiency and reliance on rare elements. Computational methods, especially based on density functional theory (DFT) have been employed to accelerate the discovery of improved materials. Yet, current approaches encounter limitations due to high computational costs and the inability to cover the vast materials space through direct high-throughput screening.

Artificial intelligence (AI) approaches have been emerged to address this problem by alleviating computational burdens and providing effective descriptors for catalytic processes. However, existing AI models have given less attention to material stability and the availability of data at different levels of accuracy. Incorporating stability-focused material discovery processes becomes crucial to facilitate efficient materials space exploration. Overcoming this challenge requires integrating information from various fidelities through multi-fidelity modelling and developing interpretable AI models.

We aim to overcome the limitations of current materials discovery approaches by employing an advanced artificial intelligence (AI)-guided workflow combined with highly accurate non-local density-functional-theory (DFT) calculations (Figure 1). For this, we plan to use the HLRN resources to perform first-principles calculations over 5000 transition metal oxides to benchmark the computational methods of transition metal oxides. These systems are chosen as they hold immense potential for applications such as photovoltaics and catalysis, but conventional local DFT methods fail to provide accurate descriptions of their properties. In particular, we will be investigating the thermodynamic as well as aqueous stability of the oxides along with their electronic properties. Our primary objective is to develop an active-learning AI approach that effectively utilizes data with different levels of accuracy to identify promising materials. To achieve this, we will leverage the power of the symbolic-regression sure-independence-screening-and-sparsifying operator (SISSO) AI approach. SISSO not only models materials properties using limited high-accuracy data but also provides valuable insights into the key physical parameters that correlate with these properties. Our proposed workflow will integrate DFT calculations, AI techniques, and efficient data management to streamline the materials discovery process. Through our AI-driven workflow that harnesses data from various levels of accuracy, we will demonstrate a cost-effective and efficient approach to the discovery of oxides with enhanced properties.

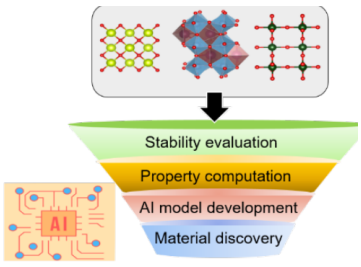

***Figure 1:** Proposed AI-workflow for oxide discovery*

WWW

https://nomad.fhi.mpg.de/

More Information

[1] Purcell, T.A.R., Scheffler, M., Ghiringhelli, L.M. et al. *npj Comput. Mater.* **9**, 112 (2023). doi: 10.1038/s41524-023-01063-y

[2] Fare, C., Fenner, P., Benatan, M. et al. *npj Comput. Mater.* **8**, 257 (2022). doi: 10.1038/s41524-022-00947-9

DFG Subject Area

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