

AI-Guided Discovery of Large-Band-Gap Dielectric Materials for Next-Generation Power Grids

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Context and Research Goals

Future energy systems will require electrical grids capable of operating at higher voltages and power densities as renewable energy sources are increasingly integrated into the network. Reliable dielectric materials are essential for high-voltage insulation in power electronics, cables, and grid infrastructure. Oxide materials, for example, HfO_2 , with a large electronic band gap are widely used for such applications due to their chemical stability and excellent insulating properties. However, discovering improved dielectric materials through conventional experimental or computational trial-and-error approaches is time-consuming and computationally expensive.

This project aims to develop a data-driven workflow to accelerate the discovery of large-band-gap oxide materials for dielectric applications. Using materials data from the Materials Project database, the student will investigate how chemical composition and atomic-scale descriptors influence electronic properties such as band gap. Machine-learning models will be developed to predict band gap values and identify key structure–property relationships. The resulting models will be used to construct a materials design map highlighting promising candidate materials for next-generation electrical insulation.

Computational and HPC Aspects

The project combines materials informatics, machine learning, and high-throughput computational materials modelling. Large datasets of oxide materials will be retrieved from the Materials Project database using Python-based programmatic access tools. Materials descriptors will be generated using materials informatics libraries such as Matminer, and machine-learning models will be trained to analyse structure–property relationships across large materials datasets.

To complement the available database information, the project will also introduce simple high-throughput first-principles calculations to estimate any missing dielectric properties and incorporate them into the dataset (automated scripts for these calculations are already available). These calculations can become computationally demanding when applied across multiple candidate materials, making high-performance computing (HPC) resources essential. The project will make use of HPC facilities available at the University of Liverpool.

By combining large-scale materials datasets, machine-learning models, and high-throughput computational screening, this project demonstrates how HPC-enabled approaches can accelerate the discovery of advanced dielectric materials for future energy infrastructure.

By the end of the project, the student will gain practical experience in Python programming, machine learning, Linux-based computational workflows, and basic HPC usage in the context of computational materials science.