Master/Bachelor Thesis:

Karlsruhe Institute of Technology
Institute of Nanotechnology

Bayesian Optimization of High-Entropy Photocatalysts

Functional materials for modern applications often need to fulfill very specific tasks, thus requiring a high degree of flexibility in adjusting their properties. This often necessitates exploring highly complex material classes that offer numerous tuning parameters, such as the choice of elements or adjustability of stoichiometries through the incorporation of various elements. However, the high complexity results in an almost infinite number of possible compositions, necessitating methods that either narrow down the parameter space or provide robust models with a limited amount of data. These models can in turn predict high-performance material compositions.

In this project, we aim to apply a machine learning/AI based approach, namely Bayesian Optimization, to optimize a highly complex material class known as high-entropy materials with respect to a specific property. The intended application for this material class is photocatalysis. In the context of photocatalysis pursued here, water is split into H2 and O2 by a catalyst activated by light. The catalyst initiates the process when light strikes the interface between water and the catalyst. Developing efficient photocatalysts could significantly support the production of hydrogen as a sustainable energy carrier.

Practically, the project involves synthesizing high-entropy materials using a high-throughput synthesis robot and analyzing their light absorption through automated UV/Vis analysis. The obtained data will be evaluated using Bayesian optimization. The Bayesian optimization approach will iteratively generate suggestions for subsequent experiments, gradually approaching optimal optical properties for photocatalysis. In this regard, the composition and stoichiometry of a high-entropy material that includes five different elements will optimized; therefore, the best-performing composition of five elements will be searched from a pool of 7-10 possible elements. The most promising developed materials will be directly applied in photocatalytic experiments to screen their performance.

Prerequisites for the master's thesis include basic programming skills (preferably Python). Familiarity with ML and AI methods would be advantageous but can also be acquired during the course of the thesis work.

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