NAWI
National Alliance
for Water Innovation

Machine Learning Platform for Catalyst Design

Anubhav Jain | Lawrence Berkeley National Laboratory (LBNL)   ajain@lbl.gov

Challenge

The current state of the art for nitrate removal from water streams is biological treatment; however, biological processes are expensive, operationally challenging, and require significant amounts of land. Developing a novel catalyst to selectively and precisely remove these constituents may offer a more cost-effective treatment alternative to the state-of-the-art. However, a major challenge with developing new catalysts is identifying a material composition that not only can react with and remove the constituent of concern, but do so quickly, and in a cost-effective manner. While researchers have traditionally taken the "brute-force-method" approach by using heuristics to identify viable electrode materials, there are a seemingly endless number of material combinations possible making this approach time consuming and highly inefficient.

Research Approach

This project will develop a high-throughput computational platform for identifying novel electrode materials using state-of-the-art user facilities at Lawrence Berkeley National Lab that integrates machine learning, high fidelity simulation, and combinatorial experimental screening. This approach has been applied to materials discovery in other fields (such as batteries and sorbents), however, it has not been systematically developed for the diverse feed stream compositions in water and wastewater treatment.

The project focus will be on applying these tools for catalysis discovery for electro-reduction of nitrates, selenium, and boron. Newly discovered materials formulations will be then synthesized via combinatorial approaches and their basic properties characterized and correlated with electrocatalytic activity and selectivity.

Impact

If successful, this project will demonstrate the viability of a new, computational, materials-screening platform that can identify potential new materials of interest that exceed the performance of commercial materials. The subsequent development of new materials that can selectively remove

nitrate, selenium and boron would not only allow existing desalination processes to operate at higher recovery, leading to more cost-effective desalination, but could also enable desalination where it currently isn't possible because the presence of these constituents makes desalination cost-prohibitive.
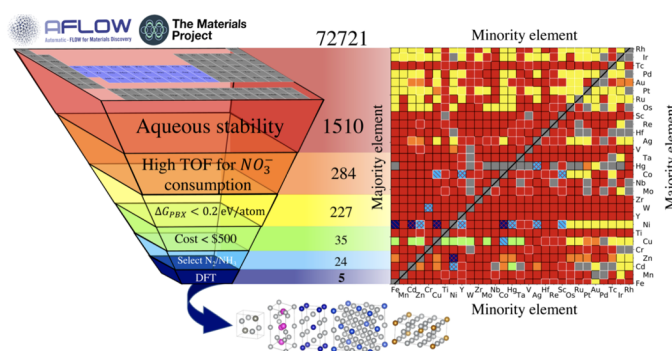
Figure 1. Machine-learning assisted computational screening is used to filter tens of thousands of potential chemical compositions and crystal structures to determine the best catalysts for nitrate removal.
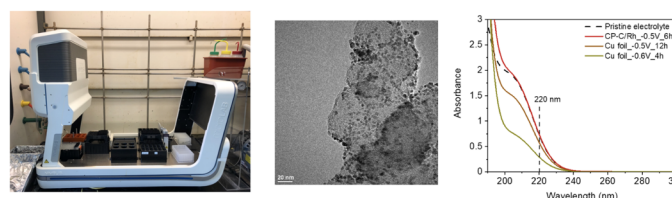
Figure 2. NIMBUS robot at Molecular Foundry for rapid synthesis of chemical compositions from computational screening; micrograph of successful nanoparticle synthesis and loading onto an electrode; development of UV-Vis technique for measuring nitrate removal.

REFERENCES

1. Tran, R.; Wang, D.; Kingsbury, R.; Palizhati, A.; Persson, K. A.; Jain, A.; Ulissi, Z. W. Screening of Bimetallic Electrocatalysts for Water Purification with Machine Learning. J. Chem. Phys. 2022, 157 (7), 074102. Link here.

U.S. DEPARTMENT OF ENERGY   Office of ENERGY EFFICIENCY & RENEWABLE ENERGY