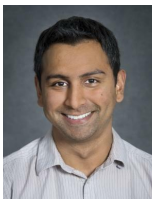
RESEARCH BRIEF
Start Date: Oct 1 2020 | Duration: 15 months

NAWI National Alliance for Water Innovation

Machine Learning Platform for Catalyst Design



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Challenge

The current methods for nitrate removal from water such as ion exchange, reverse osmosis, and biological treatment suffer from some combination of being expensive, operationally challenging, and land intensive. 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 and selenium. 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 and selenium 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.

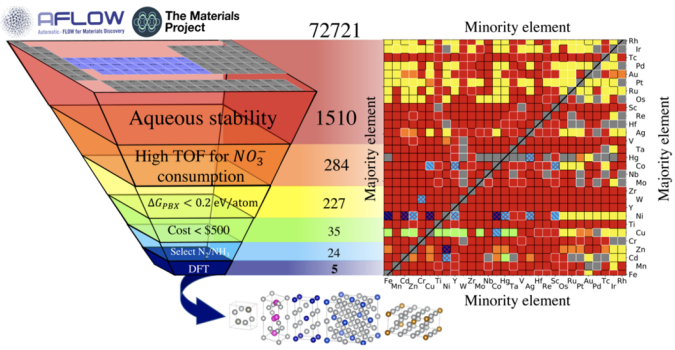

Figure 1. Machine-learning assisted computational screening is used to filter tens of thousands of potential chemical compositions and crystal structures to determine the best catalysts for nitrate removal.

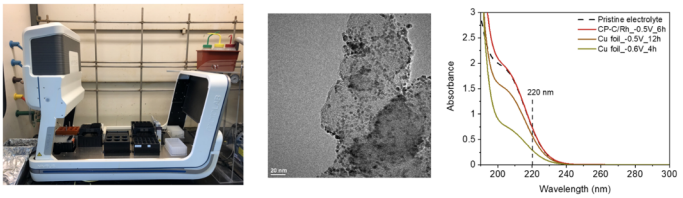

Figure 2. NIMBUS robot at Molecular Foundry for rapid synthesis of chemical compositions from computational screening; micrograph of successful nanoparticle synthesis and loading onto an electrode; development of UV-Vis technique for measuring nitrate removal.

This work was supported by the National Alliance for Water Innovation (NAWI), funded by the U.S. Department of Energy, Energy Efficiency and Renewable Energy Office, Advanced Manufacturing Office.

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Accomplishments & Findings

This project (one of NAWI's first year "Seedling" projects designed to establish foundational R&D capabilities) achieved a lot in its 15 months of operation. Our goal was to identify, synthesize and test new alloys that could electro-catalytically reduce nitrate in water to N2 or ammonia and that were: 1) stable in water; 2) showed potentially high turnover frequency for NO3-; 3) a large number of potentially active sites, and; 4) a cost of less than $500/kg (compared to $30,000/kg for Pt-based alloys). Prior work by Goldsmith et al [ref] mapped out the major reaction pathways for catalytic reduction of nitrate and provided us a head start on methods to predict how different alloys would perform as electro-reductive catalysts.

We further evaluated and refined the theoretical framework for identifying promising alloys and used NREL's EAGLE supercomputer to screen nearly 60,000 candidate alloys – many of which had never been synthesized. We initially found that Ni-based alloys seemed to have promising potential, but, after refining our theoretical methods, we changed course and eventually found that a number of copper-based alloys appeared to fit the bill. Copper alloys had been known to have potential as an electrocatalyst for nitrate reduction, but our study identified a number of new alloys that look particularly good.

We made some progress in synthesizing candidate alloys but we didn't get as far as we had hoped. Some candidate compounds were not easily synthesized, and others showed the potential for deleterious reactivity. We are currently in the process of writing up some of the experimental results for journal submission and can provide more information to interested researchers.

Related Accomplishments

There were major improvements in the tools and resources for theoretical materials screening and discovery. Machine learning (ML) approximations to complex DFT simulations are becoming reliable research tools, and the Open Catalyst Project has strengthened ML-based tools for screening compounds. COVID hurt our efforts, particularly on the synthesis side of the project due to facility closures and inability to train new staff for long periods of time.

Opportunities for Further Research

Discovering new, high-performing, low-cost electrode materials for water treatment through computational modeling and screening is a practical reality. Any water treatment technology that utilizes electro-oxidative, -reductive, or catalytic processes could benefit from using this method to explore a much wider range of potential materials that would be possible through conventional materials synthesis "trial and error". We are now applying this approach to identifying promising materials for the electrochemical removal of selenium in water in another NAWI project.

Publications and Reports

1. Tran, R.; Wang, D.; Kingsbury, R.; Palizhati, A.; Persson, K. A.; Jain, A.; Ulissi, Z. W. Screening of Bimetallic Electrocatalysts

REFERENCES

1. https://pubs.acs.org/doi/abs/10.1021/acscatal.9b02179
2. https://opencatalystproject.org/

RESEARCH PARTNERS

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