

# Direct Electrochemical Reduction of Selenium to Achieve A-PRIME Water Treatment

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## Challenge

Aquatic selenium (Se) pollution is closely associated with mining, agricultural irrigation, hydraulic fracturing, and thermoelectric power generation and is typically discharged into the aquatic environment at a ppb to ppm level as Se(IV) and Se(VI) oxyanions (e.g.,  $\text{SeO}_3^{2-}$  and  $\text{SeO}_4^{2-}$ ). To effectively mitigate aquatic Se pollution, more than 30 full-scale biological and physicochemical Se treatment processes have been implemented in North America between 2007 and 2018.<sup>1</sup> Disadvantages of existing solutions include: a large footprint, constant chemical dosing, susceptibility to performance upsets, the potential to generate toxic hydrogen selenide and organic Se species with significantly higher bioavailability (2-3 orders of magnitude) and toxicity<sup>2,3</sup> than inorganic Se, high costs, and generating large amounts of (bio)solids that require further management and may cause secondary pollution. The development of next-generation treatment systems that can precisely separate Se from complex waste streams and overcome existing challenges, may enable pipe-parity and the reuse of waters traditionally considered waste streams.

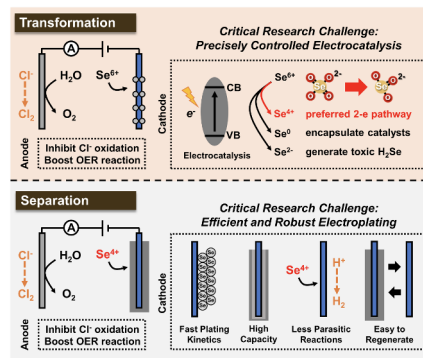
## Research Approach

In a previously funded NAWI project, the research team developed a high-throughput (HT) computational platform to screen tens of thousands of material combinations for cost-effective nitrate-reducing catalysts, ultimately leading to the identification of potentially new and cost-effective catalysts that are under experimental investigation. This new project will leverage this HT computational platform to screen and develop novel catalysts for Se reduction. The research plan is split into 3 phases:

1. Phase 1 focuses on establishing baseline performance metrics for Se electroplating and reduction, and the screening for materials that surpass the baseline.
2. Phase 2 focuses on integrating these materials into a functioning reactor.
3. Phase 3 focuses on optimization of the system to minimize side reactions, evaluate the system in realistic water matrixes, and perform a technoeconomic analysis to evaluate pipe-parity.

## Impact

This research project will leverage national lab resources such as the National Energy Research Supercomputing Center, Advanced Light Source, and Molecular Foundry for computational, experimental, and characterization to advance our fundamental understanding of Se(IV) and Se(VI) reduction mechanisms and promote a broader understanding of how electrochemical systems can be tailored for high performance. Integration of these new design techniques will constitute a unique research foundation for materials development in NAWI, enabling a new, high-throughput approach for materials design that benefits water treatment applications.



**Figure 1.** Critical challenges in transformation and separation to be addressed in this research.

## RESEARCH PARTNERS

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