RESEARCH BRIEF
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NAWI National Alliance for Water Innovation

Precise Electrochemical Dehalogenation of Halogenated Compounds in Desalination Concentrates by High Entropy Catalysts

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Challenge

Water reclamation in municipal and industrial sectors by membrane technologies concentrates halogenated organic contaminants (PFAS, antibiotics, chlorination byproducts) that pose significant health concerns. The presence of the concentrated organohalides inhibit further water recovery from and use of the retentate solution due to current and expected quality water regulations. This project aims to develop Pd-based high entropy catalysts (HECs) to achieve highly selective capture and reductive destruction of halogenated pollutants in desalination concentrates. Although PdOx catalysts achieve moderately selective capture and removal of PFAS, their cost effectiveness is too low for industrial use.

Research Approach

We will increase the Electrochemical Reductive (ER) reactivity of PdOx or Pd by doping multiple elements to form high entropy metal and metal oxide alloys, i.e., high entropy catalysts (HEC). The challenge in HEC, however, lies in selecting the right combination of four or more elements in the right proportions, which direct the reactions down the desirable pathway at a cost-effective price point. Here, we will exploit computational approaches to ascertain selective combinations, thus accelerating HEC development and couple it with reactor design construction, both directed by TEA to achieve low-cost, effective halogen removal. To promote commercialization, we aim to prove that the Pd-based HEC catalytic system developed in this project is not cost-prohibitive. The investigation of material costs of optimized electrodes, energy consumption, and service life will be the groundwork of techno-economic analysis.

RESEARCH PARTNERS

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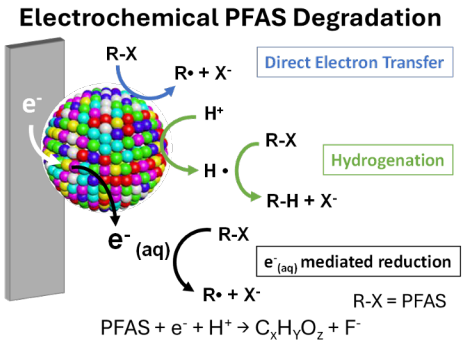

Impact

We expect the HEC-based ER system to have three distinct advantages for organo-halide treatment over existing EO and single/bi-metal catalysts: 1) the ER process is solely electric, eliminating the need for chemical addition, and does not form the oxidation species seen in EO. Compared with the EO process, the ER approach will not oxidize salt components to chlorine and bromine, which excludes the formation of organo-halide byproducts and oxyanions. 2) A single HEA particle can include multiple active centers with different functionality (e.g., Pd for C-F capture and activation, Cu for electron transfer, and Ni for hydrogen atom production). Upon investigation via the integration of experimental and computational approaches, multiple functional sites will be tailored to provide high activity for the varied elementary steps along the pathway of reduction of PFAS and chlorinated contaminants. 3) the HECs are expected to be highly stable due to their high configurational entropy, which prevents dissolution and catalytic restructuring. The configurational entropy stabilization may allow for the use of low-cost active metals which are unstable in their non-HEC forms, thus lowering overall costs. The HEC will be embedded in an inert but cathodically conductive TiO_2 matrix to gain excellent mechanical strength. In addition, HEA operated under cathodic currents will not be subject to oxidative corrosion and metal leaching. Overall, the insights gained will build a holistic knowledge framework for electrochemical dehalogenation and open the water treatment catalysts community to HEC and provide a cost-effective treatment platform for dehalogenation.

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