

## II.F.4 Hydrogen Production – Increasing the Efficiency of Water Electrolysis (New Project)

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### Objectives

Improve the operational efficiencies of electrolyzer cells operating at high current densities (i.e., high hydrogen gas production rates) by:

- Preparing and evaluating molybdenum macrocycle electrocatalysts for hydrogen evolution by water reduction in alkaline solution, and
- Preparing and evaluating a hydroxyl ion exchange membrane that primarily conducts hydroxyl ions for use as solid polymer electrolyte in alkaline water electrolysis cells.

### Technical Barriers

This project addresses the following Hydrogen Generation by Water Electrolysis barriers and General (Cross Cutting) Hydrogen Production barriers from the Hydrogen Production section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- Q. Cost
- R. System Efficiency
- Z. Catalysts

### Approach

The objectives of this project focus on developing electrocatalysts and a polymer electrolyte that improve the efficiency of the alkaline water electrolysis cell since the overriding cost element is that of the electrical energy used to run the electrolyzer. Operational efficiencies in the electrolysis of water depend on the activities of the electrode catalysts for both water reduction and oxidation at the cathode and anode, respectively, as well as the conductance of the electrolyte separating the electrodes. Development of a cathode catalyst based on molybdenum, a non-precious metal that exhibits efficient electrocatalytic activity for the hydrogen evolution reaction, is the focus of one activity. The other aims to develop a solid polymer electrolyte that conducts hydroxyl ions and will perform as the alkaline electrolyte analog to the proton exchange membrane (PEM).

We are employing several routes to forming high surface area catalysts based on a molybdenum macrocycle, e.g., Mo phthalocyanine (MoPc):

- Pyrolysis of MoPc adsorbed on monodisperse, micron-sized beads that serve as a template that is later removed;
- Pyrolysis of MoPc adsorbed on various types of carbon blacks (carbon particles); and
- Formation of a polymeric phthalocyanine structure containing molybdenum ion as the catalytic site.

By using a molybdenum complex that is polymerized or bound to a porous substrate, dissolution of the catalytic species is prevented. These electrocatalysts will be evaluated electrochemically through their performance in generating hydrogen gas from a typical alkaline solution and their resulting efficiencies.

The second task focuses on developing a novel ionically conductive hydroxyl ion exchange membrane (HEM) that could lead to improvements in cell efficiencies by increasing the overall cell conductance. This polymer that we seek to develop for improved membrane conductance consists of two features: (1) cationic sites that will promote mobile anion population and transport through the separator membrane, and (2) organized, straight channels between faces of the membrane that consequently provide the shortest-path distance between electrodes for the transport of hydroxyl ions generated at the cathode and consumed at the anode. The second feature is sought by processing diblock copolymers so that the blocks phase segregate into a structure consisting of an array of rods surrounded by a matrix, and the first by quaternizing amines in one of the polymer blocks. After preparation, the films' properties will be characterized to determine their potential success as HEMs. The resultant material must meet several criteria (including ionically conducting but electronically insulating; and chemically, electrochemically, and mechanically stable) and must perform at temperatures up to 80°C, where the efficiency of the cell is higher. Once a novel material has been identified that satisfies these criteria, a membrane electrode assembly will be fabricated and evaluated.