Center for Electrocatalysis, Transport Phenomena, and Materials (CETM) for Innovative Energy Storage EFRC Director: Grigorii Soloveichik Lead Institution: General Electric Global Research

Mission Statement: To develop the fundamental basis for an entirely new high-density energy storage system that combines the best properties of a fuel cell and a flow battery.

The basis of the organic fuel cell/flow battery system concept is a simple idea: instead of common approach of dehydrogenating an organic liquid carrier in a catalytic reactor to generate hydrogen gas and feed it to a hydrogen-air PEM fuel cell, CETM proposes to feed the hydrogenated organic liquid carrier directly into the fuel cell where it will be electrochemically dehydrogenated to a stable, hydrogen depleted organic compound without ever generating H₂. As with common hydrogen-air fuel cells, this new system will reduce oxygen from air at the cathode. The spent organic carrier may be replenished either by mechanical replacing with the fresh hydrogenated carrier at a refueling station or by electrochemically charging using protons from water electrooxidation.



CETM has identified three major research challenges in electrocatalysis, transport phenomena in membranes, and material compatibility to make this concept a reality. The selection of organic carriers suitable for organic fuel cell/flow battery is based on thermodynamic and kinetic factors central to hydrogenation and reversible dehydrogenation reaction mechanisms and is assisted by computational modeling.

Understanding of the electrodehydrogenation and electrohydrogenation catalysis is critical for realization of the organic fuel cell/flow battery concept. A good electro(de)hydrogenation catalyst should combine an effective (de)hydrogenation activity with an ability to mediate transport of two protons and two electrons per unsaturated C=X bond. Because only a few examples of catalysts for electrohydrogenation and electrodehydrogenation of organic heterocycles are known, promising leads from among the following classes of catalyst are being explored: i) catalysts for activation of the C-H bonds, ii) catalysts for hydrogenation of imines and carbonyl bonds, iii) catalysts for hydrogenation of arenes, particularly heteroarenes, and iv) catalysts that can reduce water to H₂. The emphasis will be made on non-precious metal complexes and materials.

Various strategies are being explored for attaching electrodehydrogenation/ hydrogenation catalysts to electrode materials with an emphasis on chemically robust attachments and rapid transfer of electrons and protons between the electrode and the catalyst. The coverage of the catalyst on the surface of the electrode material, its electron storage capacity and electron transfer between the electrode and the catalyst of the catalyst is studied to identify any limitations placed on the electrodehydrogenation and electrohydrogenation activities.

To develop a novel low-humidity proton exchange membrane, it is necessary to study the transport phenomena in the bulk material as a separator and the material properties needed to facilitate the convergence of charge and molecular transport to the site of the catalysis and the equally rapid removal of the products. The following major problems are being investigated: effect of the organic carriers on proton transport and membrane morphology, replacement of water with other proton conductive phase, and effect of polymer structure on membrane properties.

Since all three components of the proposed organic fuel cell/flow battery should work together seamlessly, a special emphasis will be made on fundamentals of the 3-D three-phase interface including the electrically conductive component, ion-conductive ionomer, and electrocatalyst to ensure good transport of protons, electrons, and the organic carrier in both hydrogenated and dehydrogenated forms.

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