An Interdisciplinary Approach to Developing Advanced Materials for Polymer Electrolyte Membrane Water Electrolyzers

DMREF/HydroGEN EMN Postdoctoral Position for the Tandem Development of a Comprehensive Computational Performance Model Alongside Ex-Situ Method for Investigating Materials Degradation for Low-Temperature Water Electrolysis

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This postdoctoral position may serve as an expansion of the previous work, initiated through a graduate student collaborative appointment in NREL's Electrolyzer Group. This initial research involved theoretical and practical aspects of advanced materials development for catalyst and porous transport layer (PTL) components of low-temperature polymer electrolyte membrane water electrolyzers (PEMWE). The postdoctoral position is created in the spirit of complementing the goals of the Designing Materials to Revolutionize and Engineer our Future (DMREF) and Materials Genome Initiative (MGI) programs by using complementary computational and experimental NREL HydroGEN nodes:

1. Multi-Scale Thermochemical and Electrochemical Modeling for Material Scale-Up to Component and System Design
2. Corrosion Analysis of Materials.

The computational aspect of the postdoctoral position contributes to NREL's development of a new, comprehensive model of low-temperature water electrolyzer performance under varying operational and material parameters. This postdoctoral position would focus on developing the model component related to the Ohmic overvoltage contributions from PTL and catalyst layers of various compositions and specifications under a range of operating conditions. The postdoc will utilize his/her expertise to explore the unique properties of and interactions between commonly used and newly developed materials for catalyst layer and PTL components. In particular, PEMWE performance with different combinations of materials and operating conditions can be used to investigate problematic catalytic/PTL corrosion phenomena. By addressing oversights of previous models in these areas, the new model may accelerate optimization of operating conditions and materials, with a goal of reducing the significant costs associated with PEMWE's catalytic components. Furthermore, the new computational model is designed to offer cell-to-stack and system scalability, which could further benefit the goals of HydroGEN and its collaborators.

An equal component of this postdoctoral position is an experimental investigation focusing on the phenomenon, mechanism, and performance effects of PTL and catalyst layer degradation that is commonly observed in low-temperature PEMWEs. The postdoctoral researcher would continue to validate the previously developed ex-situ electrochemical setup, designed to investigate the kinetics and mechanism of PTL material passivation. By expanding, analyzing, and refining the existing ex-situ corrosion cell testing method, catalyst components/PTLs with varying compositions, coatings, and other characteristics could be investigated under different operating conditions to improve electrolyzer performance, durability, and cost-effectiveness. The postdoctoral researcher will also be involved in the planning and initial implementation of analysis methods (including cyclic and linear sweep voltammetry and electronic impedance spectroscopy), which can serve as experimental validation of predictions made by the computational model in addition to contributing to overall goals of electrolyzer cell and stack improvement. The theoretical and experimental aspects can thus act synergistically for material advancement and scale-up.