Year 3: Identifying Cost-Effective Advanced Catalysts Using an AI-Enabled Digital Twin of a PEM Hydrogen Electrolyzer

Agarwal, Adia (School: Alexander W. Dreyfoos School of the Arts)

Hydrogen has emerged as a promising green energy storage solution due to its on-demand energy release through fuel cells. However, major barriers to wide-scale adoption remain: inefficiency and cost, specifically the reliance on precious metal catalysts such as platinum and iridium oxide. This project builds on previous research that developed an AI-assisted digital twin of a PEM (Proton Exchange Membrane) reversible fuel cell to optimize hydrogen cycle efficiency under modeled conditions. This year's work focused on identifying cost-effective anode catalyst materials for the Oxygen Evolution Reaction (OER). The model was built in MATLAB Simulink with coding assistance from Claude AI, grounded in first-principles Butler-Volmer electrochemical equations, and calibrated against Year 1 physical experimental data (baseline average efficiency: 21.64%) using a training/testing data split. An AI-enabled Python algorithm then queried the DOE Materials Project database, screening 150,000+ materials down to 30 stable transition-metal oxide candidates using elemental composition filters and a thermodynamic stability threshold (E_hull < 0.05 eV/atom). Exchange current density estimation was applied to shortlist the top 10 candidates for computational screening. All ten outperformed the Pt/C baseline, achieving efficiency gains ranging from +1.81% to +2.90%. NiFe-LDH and Fe2NiO4 produced the highest improvement at +2.90%, lowering the operating voltage by 188 mV. Co3O4 achieved a +2.20% efficiency gain at just $1.75 per gram, compared to IrO2 (the current industry-standard OER catalyst) at $141 per gram. Overall, these low-cost transition-metal oxides demonstrate significant cost-effectiveness for the future of PEM electrolyzer systems.

Awards Won: