ChatGPT

Project Context for Presentation Development

Title: Architectural Optimization of PEM Electrolyzer Catalyst Layers for Iridium Reduction

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1. Project Goals:

- **Reduce Iridium (Ir) usage by 90%** through novel catalyst layer architecture while maintaining or improving current density performance.
- **Develop a monolithic Ti-Ir architecture** using 3D printing and electrochemical deposition techniques.
- **Create digital twins of catalyst layers** to simulate and predict performance.
- **Implement AI-driven optimization** to iterate on structure-performance relationships.
- **Achieve high catalyst connectivity, mass activity, and ionic conductivity** with low contact resistance.

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2. Detailed Description:

The project proposes an architectural approach to PEM electrolyzer anode design, moving beyond conventional composition-based strategies. It introduces a digitally guided design-to-fabrication loop enabled by computational modeling and machine learning.

Workflow:

- **Digital Twin Generation**: Start with stochastic methods to recreate 3D microstructures representative of real catalyst layers.
- **Performance Prediction**: Use COMSOL-based simulations to analyze electrochemical and transport behavior of these structures.
- **AI-Driven Optimization**: Apply algorithms to modify microstructures, assess performance, and evolve towards optimal designs.
- **Fabrication**: Translate optimized structures to reality using 3D printing of titanium supports.
- **Deposition**: Coat supports with thin Ir layers through electrochemical methods.

This closed-loop framework ensures rapid development of functional catalyst layers with reduced Ir content, improved utilization, and enhanced durability.

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3. Researcher Profile (Gabriel Wosiak Leite):

- PhD in Physical Chemistry with strong emphasis on energy transition, green hydrogen, electrochemistry, multiphysical simulation and microstructural modeling.
- 1-year internship at **NREL**, sponsored by **Nel Hydrogen**, focused on multiphysics simulation and digital twin generation of PEM catalyst layers.

- Lead author of multiple high-impact publications on CFD simulation, interfacial pH analysis, and electrochemical structure optimization.
- Experienced in COMSOL, MATLAB, Python, and GAN-based digital structure generation and experimental electrochemistry.
- Invited speaker at CINE Conference; awarded for best presentation and scientific visibility.

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4. NREL Expectations and Alignment:

The **Director's Fellowship** at NREL seeks postdoctoral researchers capable of proposing bold, independent research that aligns with NREL's mission to advance clean energy technologies. NREL emphasizes:

- High scientific impact
- Cross-disciplinary innovation
- Technology transfer potential
- Data-driven solutions to energy problems

This project aligns closely with these expectations by:

- Leveraging NREL's expertise in electrochemical systems and advanced manufacturing
- Applying digital methods to reduce critical material dependency (Iridium)
- Delivering transferrable digital tools and experimental methodologies

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5. Deliverables and Impact:

- **Performance gains:** $\geq$1.5 A/cm^2 at <1.8 V
- **Volume reduction:** Catalyst layer <3 μm thick
- **Ir Mass Activity:** Targeting 0.1 A/mg
- **IP and Publications:** At least 1 provisional patent, 2+ peer-reviewed papers
- **Transferable Framework:** Modular simulation-optimization platform for other catalytic systems

This project provides a realistic, high-impact pathway to advance hydrogen production technologies and support global decarbonization goals.