Reducing electrochemical losses in solid oxide fuel cells through particle swarm optimization of microstructural polydispersity

Solid Oxide Fuel Cells (SOFCs) are energy conversion devices that efficiently transform chemical energy from fuels into electricity with minimal environmental impact. Despite their potential, widespread adoption of SOFCs is hampered by performance degradation and manufacturing challenges. A new research initiative focuses on improving SOFC efficiency by optimizing the microscopic structure of their electrodes using advanced computational and experimental methods, with a special emphasis on hierarchical materials.

The Problem: SOFC electrodes are intricate materials with multiple phases. They must balance ion and electron conduction while allowing gas diffusion to reaction sites. Key structural properties, such as particle size, shape, and distribution, influence these functions. Current manufacturing techniques often result in homogeneous microstructures that may not fully exploit the material's potential, leading to inefficiencies and long-term degradation.

Hierarchical materials, characterized by distinct structural features at multiple scales, offer a promising solution to the performance challenges of SOFCs. In this context, engineered anisotropy (directional properties) and spatially varied microstructures can optimize the competing demands for gas diffusion, conductivity, and reaction site density. By introducing varied particle sizes (polydispersity) and strategic structural organization, these materials enhance both short-term performance and long-term resilience. Hierarchical electrodes (see Figure **??** mimic natural systems, like bone or coral, where structure and function are finely tuned across scales to maximize efficiency. **The Research Goal of the project is to explore how polydispersity—or the variation in particle size and shape—impacts the performance of hierarchical SOFC electrodes.** The central hypothesis is that incorporating hierarchical features through increased polydispersity can reduce energy losses (overpotential) compared to less diverse microstructures. The **methodology** includes a dual approach:

- **Simulation and Modeling:** a Phase Field Model will predict changes in the microstructure during manufacturing, such as grain growth during sintering. Then, A *3D Transport Model* will simulate how ions, electrons, and gases move through the electrode, linking microstructural features to performance metrics like overpotential.
- **Optimization:** Particle Swarm Optimization (PSO), a computational method inspired by natural behaviors, will identify the ideal particle size distributions that maximize efficiency. Furthermore: Advanced statistical tools, including *Gaussian Mixture Modeling* and *Kernel Density Estimation*, will quantify polydispersity and measure its impact.
- **Experimental Validation:** Cells with hierarchical particle distributions will be fabricated and tested for their electrical and chemical performance. High-resolution imaging techniques - *FIB-SEM*, *PFIB-SEM* will provide detailed views of the microstructure.

The principles of hierarchical material design extend beyond SOFCs, with applications in batteries, electrolyzers, and other energy technologies. **By harnessing the advantages of multi-scale structures, this work contributes to the broader transition toward sustainable, high-performance energy systems.**

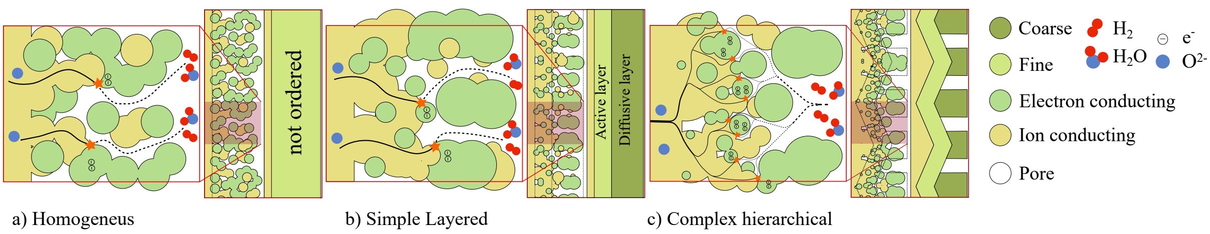

Figure 1: Hierarchy in SOFC electrodes