Machine-Learning Simulation of Oxygen Behavior in Tiny Pores for Metal-Air Battery Catalysts, and Generative-AI Design of Materials That Can Be Synthesized

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The oxygen reduction reaction (ORR) is important for clean energy technologies such as fuel cells and metal-air batteries. To improve ORR, we need to understand two things: what happens at the catalyst surface during the reaction, and how to find new materials that are both stable and actually possible to make in the lab. This work looks at both questions.

In the first part of my talk, I will talk about oxygen behavior in catalyst surface. In porous catalysts, tiny spaces (nanopores) can change how gases dissolve in water. Previous studies show that inside these tiny spaces, gas can dissolve far more than expected (an effect we call gas oversolubility) [1]. As the main reactant in the ORR, molecular oxygen may also exhibit enhanced solubility under confined conditions. Whether oxygen, the main reactant in the ORR, changes the surrounding water, is less clear. To answer this, we studied the system by using machine learning interatomic potential. This extra oxygen changes the structure of the water around it, making the water molecules more ordered near the surface [2]. These findings help explain how the local environment inside porous catalysts affects the ORR and may guide the design of better porous catalysts for fuel cells and metal–air batteries.

In the second part, I will talk about generating materials that can really be made. Recently, Microsoft released MatterGen (2025) [3], an AI model that can generate new crystal structures. However, MatterGen was trained mostly on computer-generated data. This raises a simple question: would the model do better if it learned from real experimental structures? To test this, we retrained MatterGen from scratch using experimental crystal structure data from AtomWork Advance (NIMS). Our early results show that the new model produces structures with lower energy below the convex hull, meaning the materials are more thermodynamically stable, compared with the original model trained on computer-generated data.

One study looks at how oxygen behaves inside porous catalysts; the other looks at how AI can help us find materials that are stable and can actually be synthesized. Both aim at the same goal: better materials for electrochemical energy conversion.

[1] *Journal American Chemical Society* **147** (40), 36310–36319 (2025).

[2] J. Manopo, *et. al.*, under revision in *ACS Energy & Fuels* (2026).

[3] *Nature* **639**, 624–632 (2025).