

Electrocatalyst Discovery through Advanced Synthesis, Characterization, and Data Integration

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The development of efficient and scalable electrocatalysts for energy applications increasingly demands not only innovation in synthesis but also a systematic approach to data generation and interpretation. In this talk, I will present a comprehensive overview of our strategies for preparing electrocatalysts based on metals, alloys, and high-entropy materials, emphasizing a modular and data-centric workflow.

We employ diverse synthesis methods including electrodeposition, nitridation, anodic oxidation, and laser surface structuring to tailor catalytic properties and engineer finely tuned surface chemistries. Particular attention will be given to our use of laser-based methods which enable rapid surface modification suitable for both research and industrial contexts. To understand the evolution of structure and composition at each stage, we integrate advanced characterization techniques, such as identical location scanning electron microscopy (IL-SEM), XPS, XRD, and electrochemical testing. One such example of structural and compositional complexity can be found in our recent work,¹ which highlights the multi-level complexity of such systems — ranging from material structure to collaborative workflows—and underscores the need for new, systematic approaches capable of handling and leveraging this complexity.

A key focus of our work is the interplay between experiment and data science. We harness machine learning algorithms to process large datasets, reveal hidden correlations, and guide the synthesis. Data is structured and managed through the Qx application, enabling standardized, searchable, and interconnected records across synthesis, characterization, and performance evaluation.

By combining multiple synthesis methods, advanced characterization techniques, and structured data management and analysis, we create an integrated approach that accelerates the discovery of next-generation electrocatalysts. The talk will conclude with reflections on how integrating digital tools into experimental workflows enables more systematic exploration, knowledge extraction, and informed decision-making in electrocatalyst development.

1. L. SUHADOLNIK, et al., *Materials Today Chemistry*, **2024**, 35, 101835