Chemistry Seminar

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4:00 pm at 126 Schrenk Hall

Understanding Design Principles for Electrochemically Active Interfaces: From Metal Chalcogenides to Few-Atom clusters

Bio: Amarachi Clare Nnachor is a third-year Ph.D. student in Nath Research Group where she conducts research on nanomaterials for energy applications. Her work focuses on transition metal chalcogenides and few-atom catalysts for electrocatalytic oxygen evolution and related clean energy processes. She earned her Bachelor of Science in Industrial Chemistry from Nnamdi Azikiwe University, Nigeria. Amarachi is passionate about developing sustainable materials for energy conversion and advancing innovative solutions in electrochemistry, catalysis, and nanoscience.

Abstract: Electrocatalysis provides a scalable pathway to convert chemical fuels into renewable energy and value-added products. However, implementation is limited mostly due to the rising cost and scarcity of precious metals feedstock. Although recently transition metals have been studied for electrocatalytic activities, the existing knowledge gap for composition-structure-activity relationships for earth abundant transition elements under operating conditions needs to be addressed.

This work combines controlled materials synthesis, rigorous electrochemical testing, and density functional theory (DFT) studies to probe and design catalytically active sites in transition metal-based electrocatalysts, ranging from chalcogenides to coordination-defined few-atom metal clusters supported on graphene

In the first part of this talk, phase and stoichiometry control in Ni and Mn based selenides is used to tune morphology and electronic structure, enabling systematic evaluation of electrocatalyst efficiency for oxygen evolution reaction (OER) in alkaline media. Performance is quantified through electrochemical benchmarking including overpotential, Tafel analysis, impedance, and durability tests paired with post-reaction characterization to connect activity trends to composition, nanostructure, and metal center identity.

Finally, active-site design is extended beyond bulk phases by introducing few-atom metal clusters anchored on biowaste derived N-doped graphene. These platforms allow d-electron density, anchoring chemistry, and electrolyte environment at the catalytic site to be tuned to control interfacial charge transfer and oxidation pathways. DFT slab models and adsorption energetics are used to relate local coordination environments to key intermediates (e.g., *OH), enabling mechanistic interpretation and guiding selection of composition and surface termination.