Clarkson University
Department of Chemical and Biomolecular Engineering
SEMINAR (Graduate Student Presentation)

"Understanding Alloy Behavior Towards Optimal Electrocatalytic Design"

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Electrocatalysis is a growing field of research that holds great potential as a sustainable route for advancing various technologies and improving their efficiency and economic viability. The discovery of systems that can break adsorption energy scaling relations can provide important insight into electrocatalytic design. Recent investigations have begun to elucidate the possibilities of alloy surfaces in breaking linear relationships between adsorption energies due to their distinctive characteristics. They possess multiple metallic elements with varying electronic structures and properties, which can promote a diverse range of reaction pathways leading to a disruption of the scaling relations observed in pure metals. In addition, the presence of different metals in an alloy can create synergistic effects that enhance the catalyst's activity and selectivity for specific reactions.

My research focuses on understanding the fundamental mechanisms of alloys and exploring how they can be designed to break the adsorption energy scaling relations with the aim of achieving optimal electrocatalytic systems. Computational methods, such as density functional theory (DFT), can provide valuable insights into the alloy's electronic and surface properties. By understanding the behavior of alloys, it is possible to adjust their composition and electronic structure to improve their electrocatalytic performance. Preliminary results have demonstrated some of these unique properties of alloy catalysts in a limited number of cases. Selective step decoration, a novel approach, has also shown the potential to break scaling relations by modifying the electronic and geometric properties of catalyst surfaces. Further studies and investigations are necessary to fully understand how to redesign alloy catalysts, break or modify scaling relations, and produce catalysts that offer significantly improved activity, stability, and selectivity.

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CAMP 175

Onyinyechukwu Goodness Njoku is a Ph.D. student at Clarkson University, where she works under the supervision of Dr. Ian McCrum. Her research focuses on using Density Functional Theory (DFT), a computational modeling method, to gain insights into electrocatalysis and surface science at the atomic level. Before joining Clarkson University, Onyinyechukwu earned a BTech degree in chemical and petrochemical engineering from Rivers State University in Port Harcourt, Nigeria.