



SCHOOL OF
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College of Engineering, Architecture and Technology

CHE SEMINAR SERIES

Digital Catalysis for Sustainable Electrochemical Processes

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Achieving a sustainable energy future is critical to overcoming the ever-increasing energy demands, reducing our dependence on conventional energy sources based on fossil fuels, and impeding climate change. One aspect of this grand challenge involves developing sustainable energy storage and conversion electrochemical processes to convert electricity into fuels and chemicals, as renewable energy sources (solar, wind, and hydroelectric) are intermittent. Electrochemical processes provide a unique set of parameters to optimize catalyst material, reaction environment, and process performance. Oxygen electrocatalysis remains the bottleneck of the efficiency of Proton exchange membrane (PEM) fuel cells and electrolyzer devices due to sluggish reaction kinetics, high cost, and scarcity of catalytic materials. In addition to material discovery efforts, understanding the solid-liquid interface especially the effects due to acid electrolyte anions and pH is crucial to designing and optimizing existing electrocatalysts under diverse electrochemical microenvironments. In this talk, I will first describe our efforts to accelerate material discovery by accounting for both material stability and activity for oxygen-based electrochemical reactions. Next, I will discuss our efforts to systematically study the effect of acid electrolytes on oxygen electrocatalysts. Finally, I will discuss the microkinetic model we developed by incorporating the effects of the electric field under oxygen electrocatalyst reaction conditions to predict and compare the onset potentials, 2e vs 4e activity, Tafel slopes, and pH effects with experiments. The expansion of next-generation oxygen electrocatalysts discovery by accounting for both stability and activity and fundamental understanding of the effects of acid electrolyte anion adsorption and pH assists in engineering better-performing catalysts with integrated microenvironments for oxygen electrocatalysis and other sustainable electrochemical processes.

NORTH CLASSROOM BUILDING 203

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Kasun Gunasooriya is an assistant professor of Sustainable Chemical, Biological and Materials Engineering at the University of Oklahoma. He received his B.Eng. and M.Eng in Chemical Engineering from the National University of Singapore (NUS) and earned his Ph.D. (2019) in Chemical Engineering from the Laboratory for Chemical Technology (LCT)

at Ghent University, Belgium. Kasun completed his postdoctoral research in Catalysis Theory Center at the Technical University of Denmark (DTU). His research efforts are aimed at developing materials and processes to produce renewable energy, fuels, and chemicals with improved efficiency and durability that can benefit societal and economic growth while minimizing impacts on the environment. In pursuit of these goals, he combines the fields of computational catalysis, kinetic and continuum modeling and machine learning to investigate complex and dynamic catalytic materials, reaction environments and processes, and techno-economic and lifecycle analysis to improve economic feasibility and minimize the environmental impact of sustainable technologies. He received ORAU Ralph E. Powe Junior Faculty Enhancement Award, Young Talent Award from the International Congress on Catalysis, 1st prize in the European Federation of Catalysis Societies (EFCATS) Young Generation Catalysis Challenge, and an invitation to give a TEDx talk entitled 'Hacking the carbon cycle using computers'. He serves as a Young Advisory Board member in Applied Catalysis A: General journal.

