Atomic-scale nanomaterials design for sustainable energy development

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Chemistry Seminar on *Computational Design of Electrocatalyst*

Monday Jan. 29 at 4 pm in 303 Schrenk

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Abstract: Electrocatalysis is a key technology for sustainable energy development, as it can enable energy storage from intermittent renewable sources. To design high-performance electrocatalysts, we need to understand the atomic structure and chemistry of the nanomaterials and their active sites. The active sites of electrocatalysts are dynamic at the electrode-electrolyte interface, undergoing structural transformations, valence state changes, and coordination environment alterations during reactions. These changes are affected by various factors, such as solvent, pH, electrolyte, and applied bias potential. Computational materials science can help us investigate the electronic properties of active sites at the atomic level under different operational conditions, providing valuable insights into the mechanisms of electrocatalytic reactions and helping us optimize the electronic properties of active sites of catalysts for improved energy conversion efficiencies. In this talk, I will show how we can computationally control the electronic properties of nanomaterials by engineering their composition, atomic structures, and external factors, leading to the data-driven molecular design of high-performance functional nanomaterials for sustainable energy applications.

About the speaker: Dr. Yun Wang is an Associate Professor at Griffith University and a Fellow of the Royal Society of Chemistry. He is an expert in computational materials science, with a focus on catalysis and renewable energy. He has published about 200 papers in high-impact journals, such as Nature and Nature Energy. His research aims to understand and control the electronic properties of nanomaterials for green chemistry technologies.