**Announcing the Final Examination of Kaige Shi for the degree of Doctor of Philosophy in Physics**

**Date:** October 30, 2024

**Time:** 10:00 a.m.

**Room:** PSB 160

**Dissertation title:** Elucidating the Effects of Cations and Electrode Wettability on Electrocatalysis

**Abstract:**

Electrocatalysis plays a key role in the development of energy conversion technologies including fuel cells and electrolyzers, which can enable sustainable production of chemicals and fuels when powered by renewable electricity. Beyond electrocatalytic materials, the local environment around the catalyst, such as liquid electrolyte and gaseous reactant/product, has a significant effect on electrocatalytic reactions such as CO2 reduction and hydrogen evolution. This dissertation focuses on understanding the effects of electrolyte cations and electrode wettability on the reaction kinetics and bubble dynamics of electrocatalytic reactions. First, I studied the effect of non-metal cations including ammonium and alkylammonium on CO2 reduction with Bi catalyst, which showed a significant improvement of CO production as compared to that with alkali metal cations, but a minor one on formate production. This is because the cations play a critical role by stabilizing the \*CO2 intermediate for CO production, which is however not necessary for formate. Based on the understanding, I further investigated the cation effect on CO2 reduction with Au using gas-diffusion electrodes, which achieved a multi-fold enhancement of CO production activity using ammonium cations. The ammonium-based cations also exhibited a significant promotion of the hydrogen evolution in neutral electrolyte, which is attributed to a proton-shuttling mechanism enabled by the cations with proton-donating abilities. On the other hand, I investigated the effect of electrode wettability on gas-evolving electrocatalysis by tuning the wetting properties with O- or F-doped carbon supports to make it hydrophilic/hydrophobic, which both improved the activity as compared to pristine carbon support. The hydrophilicity increases the exposure of catalyst surface to liquid electrolyte, while the hydrophobicity accelerates the bubble dynamics of generated N2 and recovery of the active sites. The research here provides new fundamental understanding of the effects of electrolyte cations and electrode wettability on electrocatalysis as well as insights for the rational design of efficient electrocatalytic systems for renewable energy applications.

**Outline of Studies:**

Major: Physics

**Educational Career:**

B.S., 2018, Southern University of Science and Technology

**Committee in Charge:**

Dr. Xiaofeng Feng (Chair)

Dr. Talat Rahman

Dr. William Kaden

Dr. Xiaohu Xia (External Committee Member)

Approved for distribution by Xiaofeng Feng, Committee Chair, on October 03, 2024.

The public is welcome to attend.