CHEMICAL ENGINEERING
COLLEGE OF ENGINEERING AND APPLIED SCIENCE

SUMMER RESEARCH OPPORTUNITIES FOR UNDERGRADUATE students

FOR APPLICATION YEAR: 2024

PROJECT TITLE: Machine learning-assisted catalyst design for CO2 Conversion

Jingjie Wu
Chemical Engineering
578 MC
wu2jj@ucmail.uc.edu
Phone: 513 556 2756

Project Description

Electrochemical conversion of CO2 from flue gas or direct air capture to platform chemicals at ambient conditions can potentially displace petroleum-based chemical production in a low-carbon economy when coupled with renewable and affordable electricity. Copper (Cu) is the unique known metal catalyst that is capable of catalyzing CO2 electro-reduction (eCO2RR) into C2+ chemicals (primarily involving ethylene (C2H4) and ethanol (C2H5OH)) and high-order C1 products (e.g., methane (CH4) and methanol (CH3OH)). However, Cu has a wide product distribution and requires relatively high overpotentials, which makes electrochemical CO2 reduction technology far from practical application.
Distinct from prior efforts focusing on the C-C coupling step, this project aims to identify the reaction descriptors describing the interaction between selectivity determining intermediate (SDI) and catalytic site via integrated experimental and density functional theory (DFT) efforts and to rationally design Cu catalysts guided by machine learning (ML) prediction to navigate the selectivity toward a C2+ single product. This project will advance the sustainable and circular manufacturing of platform chemicals using CO2 as a feedstock, consolidating efforts in precise catalyst design and synthesis, DFT modeling, and ML. Upon completing this project, the students are encouraged to build a team to participate in EnergyTech University Prize, a new Department of Energy competition with over $250,000 in cash prizes.