Yani Guan
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EDUCATION

Chemical and Biomolecular Engineering, University of California Los Angeles, Los Angeles, CA, U.S.
09/2022 – Present
Doctor of Philosophy, Major in Chemical Engineering
- Coursework: Electrochemical Systems, Electrochemistry

Chemical and Biomolecular Engineering, University of California Los Angeles, Los Angeles, CA, U.S.
09/2022 – 03/2024
Master of Science, Major in Chemical Engineering
- Coursework: Transport Phenomenon, Advanced Engineering Thermodynamics, Advanced Chemical Reaction Kinetics, Applied Mathematic Theory

Department of Chemical Engineering, Hebei University of Technology, Tianjin, China
09/2018 – 06/2022
Bachelor of Science, Major in Chemical Safety Engineering
- Honors and Awards:
  - Outstanding Award for Innovation and Entrepreneurship of College Students in Tianjin (the only student nominated for the prize in the department)
  - Second Prize of College Students Innovation and Entrepreneurship in Hebei Province
  - Youth Star in Hebei province
  - Hebei University of Technology Innovation Award (only two for undergraduates)

RESEARCH EXPERIENCE

University of California, Los Angeles   **09/2022 – Present**

Supervisor: Professor Philippe Sautet

- ◼ **Project: Probing the Electric Double Layer Capacitance**
  Intro: Understand the Reaction Environment in Conditions of Electrochemical Amination of Acetone
  - Analyzed adsorption behavior of acetone and methylamine on copper electrodes using impedance spectroscopy
  - Investigated interfacial polarizability and EDL capacitance via grand canonical DFT and ab initio molecular dynamics

- ◼ **Project: Cu-based Electrode Degradation and Stability**
  Intro: Determine the Origin of copper dissolution in electrocatalytic reduction conditions involving amines
  - Uncovered Cu dissolution mechanisms in amine solutions using Grand Canonical DFT, revealing surface restructuring even at negative potentials
  - Identified amine-driven Cu extraction and complexation as key factors in cathode degradation under electroreduction conditions

- ◼ **Project: Electrochemical Reductive Amination Reactivity**
  Intro: Study the Enhanced Electrochemical Amination of Acetone via Pb-Catalyzed Hydrogen Transfer and Imine Hydrogenation
  - Investigated Pb's role in electrochemical hydrogenation, revealing a dynamic PbH_2–PbH_4 cycle that facilitates imine reduction
  - Demonstrated Pb acts as a hydrogen shuttle, lowering energy barriers and enhancing catalytic efficiency in reductive amination
  - Extended this hydrogen shuttle effects to other post-transition metals, such as Tl, Pb and Bi

Hebei University of Technology   **12/2018 – 01/2022**

Supervisor: Professor Jingde Li

- ◼ **Project: Bifunctional Oxygen Electrocatalyst**

Intro: Reported an efficient bifunctional catalyst in ORR&OER electrocatalysis.

- Synthesized an efficient cobalt nitride hybrid bifunctional electrocatalyst, which consists of sulfur-doped, and mildly oxidized $Co_{5.47}N$ nanoparticles supported on nitrogen-doped reduce graphene oxide sheet (O-S-$Co_{5.47}N$@N-RGO).
- Studied the catalytic performance using DFT calculations.

- **Project: Multi-scale Simulation in Catalysis and Materials**
  Intro: Conducted DFT simulations in catalysis kinetic analysis using VASP program and further studied a series of dynamic simulations using first-principles-based Kinetic Monte Carlo (KMC) to study the kinetic performance of these reactions.
  - Studied the effect of oxide state and valence state on CO_2RR reaction on Cu (111) and CuO (111).
  - Simulated hydrogen evolution reaction (HER) on Pt (111) and Pt (100) to investigate the effect of surface morphology and hydrogen coverage on hydrogen production, where the curve of current during the reaction process was plotted and the influence of initial voltage on the reaction was studied.
  - Conducted methane steam reforming (MSR) on Ni (111) to understand the effect of H_2S on catalyst deactivation, where the effect of H_2S on catalyst deactivation was studied.

- **Project: Machine Learning in Heterogeneous Catalysis**
  Intro: Carried out literature research comprehensively and learned machine learning algorithm systemically. Meanwhile, practiced using mainstream frameworks to fit the data and predict experiment results based on existing databases.
  - Completed a literature review on recent developments, challenges and perspectives of ML in solid heterocatalysis.
  - Used mainstream ML frameworks, such as PyTorch and TensorFlow to practice several assignments on simulation and prediction.
  - Studied how to store, proceed, and analyze data, as well as some language processors, database management systems, and services, such as MySql and NumPy.

PROFESSIONAL EXPERIENCE

DP technology   **06/2022 – 09/2022**

Algorithm Researcher

- Facilitated project management for Hackathon 2.0 in AI for Science, developing comprehensive user documentation promoted adoption and application of tools across research and industry sectors
- Fostered community growth by addressing technical challenges (installation, compatibility, bug fixes, model tuning & opt) for 200+ global users, improving usability and impact of open-source software, including DeePMD-kit, ABACUS, and dflow

TECHNICAL SKILLS

- Programming (advanced): Python (Certified in Python for Everybody at University of Michigan), R, MATLAB, Shell Scripting
- Machine Learning Libraries (intermediate): Scikit-learn, PyTorch, TensorFlow
- Simulation and Modeling Software (advanced): VASP, LAMMPS, COMSOL, Simulink, AutoCAD

CONFERENCE

[1] Yani Guan (Presenter), Philippe Sautet, Origin of Copper Dissolution in Electrocatalytic Reduction Conditions Involving Amines, **Electrochemical Society Meeting Abstracts prime2024**, 1621-1621, Honolulu, HI

[2] Yani Guan (Presenter), Philippe Sautet, Origin of Copper Dissolution in Electrocatalytic Reduction Conditions Involving Amines, **ACS Fall 2024**, Denver, CO

PUBLICATION

[11] Guan, Yani; Kümper, Justus; Kumari, Simran; Heiming, Nick; Mürtz, Sonja D; Steinmann, Stephan N; Palkovits, Stefan; Palkovits, Regina; Sautet, Philippe; Probing the Electric Double-Layer Capacitance to

Understand the Reaction Environment in Conditions of Electrochemical Amination of Acetone. *ACS Applied Materials & Interfaces*, 2025, 17, 4087−4097

[10] Guan, Yani; Kümper, Justus; Mürtz, Sonja D; Kumari, Simran; Hausoul, Peter JC; Palkovits, Regina; Sautet, Philippe; Origin of copper dissolution under electrocatalytic reduction conditions involving amines, *Chemical Science*, 2024, 15, 14485-14496

[9] Kümper, Justus; Mürtz, Sonja D; **Guan, Yani**; Kumari, Simran; Hausoul, Peter JC; Kurig, Nils; Sautet, Philippe; Palkovits, Regina; Metallic Impurities in Electrolysis: Catalytic Effect of Pb Traces in Reductive Amination and Acetone Reduction, *Angewandte Chemie International Edition*, 2024, 63, e202411532

[8] Luo, Yuhong; **Guan, Yani**; Liu, Guihua; Wang, Yanji; Li, Jingde; Ricardez-Sandoval, Luis; First-Principles-Based Kinetic Monte Carlo Model of Hydrogen Evolution Reaction under Realistic Conditions: Solvent, Hydrogen Coverage and Electric Field Effects, *ACS Catal*. 2024, 14, 4, 2696–2708

[7] Zhao, Ximeng; **Guan, Yani**; Du, Xiaohang; Liu, Guihua; Li, Jingde; Li, Gaoran; Ordered macroporous V-doped ZnO framework impregnated with microporous carbon nanocages as multifunctional sulfur reservoir in lithium-sulfur batteries, *Chemical Engineering Journal*, Volume 431, Part 3, 1 March 2022, 134242

[6] Guan, Yani; Chaffart, Donovan; Liu, Guihua; Tan, Zhaoyang; Zhang, Dongsheng; Wang, Yanji; Li, Jingde; Ricardez-Sandoval, Luis; Machine learning in solid heterogeneous catalysis: Recent developments, challenges and perspectives, *Chemical Engineering Science*, Volume 248, Part A, 2 February 2022, 117224

[5] Guan, Yani; Suo, Wei; Zhang, Zisheng; Wang, Yanji; Sun, Shujuan; Liu, Guihua; Insights on the catalytic active site for CO2 reduction on copper-based catalyst: a DFT study, *Molecular Catalysis* 511, 111725

[4] Niu, Weixing; **Guan, Yani**; Luo, Yuhong; Liu, Guihua; Li, Jingde; A macroporous titanium oxynitride-supported bifunctional oxygen electrocatalyst for zinc–air batteries, *Catalysis Science & Technology*, 11 (24), 7922-7931

[3] Liu, Fan; **Guan, Yani**; Du, Xiaohang; Liu, Guihua; Sun, Daolai; Li, Jingde; A conductive and ordered macroporous structure design of titanium oxide-based catalytic cathode for lithium–sulfur batteries, *Nanotechnology*, 33 (12), 125704

[2] Sun, Miao; Ji, Haifeng; **Guan, Yani**; Zhang, Yue; Zhang, Xiaojie; Jiang, Xiaoxia; Qu, Xiongwei; Li, Jingde; Nanoscale melamine-based porous organic frameworks as host material for efficient polysulfides chemisorption in lithium–sulfur batteries, *Nanotechnology*, 32 (8), 085402

[1] Guan, Yani; Liu, Guihua; Li, Jingde; Wang, Yanji; Zhang, Zisheng; Surface-engineered cobalt nitride composite as efficient bifunctional oxygen electrocatalyst, *Nanotechnology* 30 (49), 495406