Yani Guan

Email: **yaniguan@g.ucla.edu**

EDUCATION

Chemical and Biomolecular Engineering, University of California Los Angeles, LA, California, U.S.
09/2022 – Present
Doctor of Philosophy, Major in Chemical Engineering

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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)

INTERESTS

Photography and Making albums; Traveling and Stamping; Video games;
Sports (Table tennis; Swimming; Badminton)

RESEARCH EXPERIENCE

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

Supervisor: Professor Philippe Sautet

- **Project: Electrochemical pyrrolidone synthesis: theoretical investigation of the electrochemical amination of levulinic acid (ElectroPyr)**

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.

PUBLICATION

[1] **Yani Guan**, Donovan Chaffart, Guihua Liu*, Zhaoyang Tan, Dongshen Zhang, Yanji Wang, Jingde Li*, Luis Ricardez-Sandoval*, Machine Learning in Solid Heterocatalysis : Recent Developments, Challenges and Perspectives. *Chemical Engineering Science*, 2022, 248, 117224. DOI: https://doi.org/10.1016/j.ces.2021.117224

[2] **Yani Guan**, Wei Suo, Zisheng Zhang, Yanji Wang, Shujuan Sun*, Guihua Liu*. Insights on the Catalytic Active Site for CO_2 Reduction on Copper-based Catalyst: a DFT study. *Molecular Catalysis*, 2021, 511, 111725. DOI: https://doi.org/10.1016/j.mcat.2021.111725

[3] **Yani Guan**, Guihua Liu, Jingde Li*, Yanji Wang, Zisheng Zhang*, Surface-engineered Cobalt Nitride Composite as Efficient Bifunctional Oxygen Electrocatalyst, *Nanotechnology*, 30, 49, 2019. DOI: https://doi.org/10.1088/1361-6528/ab4144

[4] Ximeng Zhao, **Yani Guan**, Xiaohang Dua, Guihua Liu, Jingde Li*, Gaoran Li*, Ordered Macroporous V-doped ZnO Framework Impregnated with Microporous Carbon Nanocages as Multifunctional Sulfur Reservoir in Lithium-sulfur batteries, *Chemical Engineering Journal*, 2021. DOI: https://doi.org/10.1016/j.cej.2021.134242

TECHNICAL STRENGTHS

- Programming: Python, C++
- AI frameworks: TensorFlow, PyTorch
- Software skills: MatLab, Gaussian, Material Studio, VASP, AutoCAD