LEYU LIU • 刘 乐雨

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EDUCATION

Tsinghua University (THU) Sept. 2019 - Present
Ph. D. Candidate in Chemistry, Theoretical & Computational Advisor: Hai Xiao & Jun Li

Xiamen University (XMU) Sept. 2015 - Jun. 2019
B.Eng. in Materials Science and Engineering

SCHOLARSHIPS & AWARDS

Excellent Oral Presentation Award in the 727th THU Doctoral Academic Forum	2023
Shimadzu Academic Scholarship, THU	2023
Friends of Tsinghua-Gao Yingshi Scholarship, THU	2023
Social Work Excellence Award, THU	2021
Outstanding Graduates, XMU	2019
Merit Student, XMU	2016, 2018
Excellent Academic Scholarship, XMU	2016~2018

WORK & RESEARCH EXPERIENCE

- **Theoretical Modeling of Elementary Steps in Electrochemical Reduction Reactions**
  - Mechanistic study on the interplay between the applied potential and the kinetics of CO_2 activation in electrochemical CO_2 reduction reaction (CO_2RR) using the grand canonical density functional theory (GC-DFT) method combined with the implicit electrolyte model.
  - Explicit constant-potential modeling of neutral and alkaline hydrogen evolution reaction (HER) kinetics to clarify reaction mechanisms and the origin of catalyst activity.
- **Investigation and Control of Electrochemical Interfacial Reaction Microenvironment**
  - Global optimization of adsorbate coverages and adsorption sites under electrochemical conditions using constant-potential ab initio molecular dynamics (AIMD) and the constrained minima hopping (global optimization) method.
  - Dynamic modeling of hydrogen bond networks among interfacial water molecules for catalyst design in neutral HER.

PUBLICATIONS

1. Shen, Q.; Yang, H.; Zhao, K.; **Liu, L.**; Sun, Q.; Chang, X.; Xiao, H.; Xu, B. Unraveling Intrinsic Electronic Factors in Thermocatalytic (Hemi-)Hydrogenation of Ethylene and Acetylene with Electric Polarization. *ACS Catal.* **2023**, *13*, 14570-14579.
2. **Liu, L.**; Xiao, H., Inverted Region in Electrochemical Reduction of CO_2 Induced by Potential-Dependent Pauli Repulsion. *J. Am. Chem. Soc.* **2023**, *145* (26), 14267-14275.
3. Sun, K.; Wu, X.; Zhuang, Z.; **Liu, L.**; Fang, J.; Zeng, L.; Ma, J.; Liu, S.; Li, J.; Dai, R.; Tan, X.; Yu, K.; Liu, D.; Cheong, W.-C.; Huang, A.; Liu, Y.; Pan, Y.; Xiao, H.; Chen, C., Interfacial water engineering boosts neutral water reduction. *Nat. Commun.* **2022**, *13* (1), 6260.

ADDITIONAL

- Language Proficiency: Mandarin (Native), English (Fluent)
- Professional Software: VASP, JDFTx, ASE, Quantum ESPRESSO, CP2K, Gaussian
- Programming/Scripting tool: Python, Matlab, Bash
- Other skills: System Manager of Laboratory High-Performance Computing (HPC) Server