Tianyou Mou

Chemical Engineer | Data Scientist
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Education

Ph.D. in Chemical Engineering, Virginia Tech, Grade: 3.76, 2018 – Fall 2022
B.S. in Chemical Engineering, Rutgers, The State University of New Jersey, Grade: 3.96, 2016 – 2018
B.S. in Chemical Engineering, Beijing University of Chemical Technology (BUCT), Grade: 3.60, 2013 – 2016

Experiences

Graduate Research Assistant, Xin group, Virginia Tech, Blacksburg, VA 08.2018 - present

Research #1: Understanding the mechanism of electroreduction of CO_2 on nanomaterials

- Developed methods to calculate charged and solvated heterogeneous systems. (🔗)
- Performed MD and electronic structure calculations (DFT and *ab inito* MD) for probing free energy landscapes.
- Strong solid-state physics and crystallography background helped set up the interface of the heterjunction structure of nanomaterials.

Research #2: Machine Learning (ML) of lateral adsorbate interactions in surface reaction kinetics

- Developed ML models called Cluster Expansion-Theory Infused Neural Network (CE-Tinnet) to predict lateral interactions between atoms in nanomaterials. (🔗 and 🔗)
- Applied Kinetic Monte Carlo (KMC) theory to investigate the instability and evolution of nanomaterials. (🔗)

Research #3: Monodisperse PdSn/SnOx core/shell nanoparticles with superior electrocatalytic ethanol oxidation performance

- Closely collaborated with experimental researchers and successful explained experimental phenomenon by computational electronic structure studies.

Research #4: Applying machine learning (ML) for material property prediction (🔗)

- Developed a transfer learning framework to predict material properties with less data.

Research #5: Economic analysis of N_2 electrochemical reduction to fertilizer (🔗)

- Provided a small-scale fertilizer production facility powered by clean energy to solve the world starving problem.
- Performed an economic analysis along with the Aspen plus analysis to apply the small-scale facility in suitable areas.

Project #1: Calculating the Hartree Fock energy of hydrogen using python. (🔗)

Project #2: Data mining for catalysis materials. (🔗)

Working Environment Coordinator, Xin group, Virginia Tech, Blacksburg, VA 08.2018 - present

- Trained graduate and undergraduate students (>10) for using supercomputing and operating systems. (🔗)
- Managed supercomputing working environments for Xin group including the compilation, installation, and maintenance of VASP, Quantum ESPRESSO, Bash, working modules, allocation, etc. (🔗)

Skills

- Programming languages: Python, MATLAB, Bash, HTML
- Data science tools: PyTorch, TensorFlow, NumPy, Pandas, SciPy, Scikit-learn
- Computational chemistry tools: VASP, Quantum ESPRESSO, LAMMPS, CP2K, VMD, VESTA, Chimera
- Other software: Illustrator (Ai), 3ds Max, Auto CAD, Aspen Plus, Photoshop, Video editing

Selected Publications

- **Mou, T.**, Han, X., Pillai, H. S., Zhu, H., Xin, H., (2021) Understanding the Mechanism of CO2 Electroreduction on Bi Surfaces with Ionic Liquid Electrolytes. (**Manuscript.**)
- Han, X., **Mou, T.**, Liu, S., Ji, M., Gao, Q., He, Q., Xin, H. and Zhu, H., (2021) Heterostructured Bi–Cu_2S nanocrystals for efficient CO_2 electroreduction to formate. *Nanoscale Horizons*. (**Co-first author, accepted.**)
- **Mou, T.**, Han, X., Zhu, H., Xin, H. (2021) Machine Learning of Lateral Adsorbate Interactions in Surface Reaction Kinetics. *Current Opinion in Chemical Engineering*. (**Submitted.**)
- Gao, Q., **Mou, T.**, Liu, S., Johnson, G., Han, X., Yan, Z., Ji, M., He, Q., Zhang, S., Xin, H., Zhu, H. (2020) Monodisperse PdSn/SnOx core/shell nanoparticles with superior electrocatalytic ethanol oxidation performance. *Journal of Materials Chemistry A*. 2020, 8, 20931–20938. (DOI)

Activities & Leadership

- President of the Student Union, BUCT, 2014-2016
- Volunteer of the World AIDS Day, 2014, and the Beijing International Halfway Marathon, 2015

Honors & Awards

- Hord Graduate fellowship, Virginia Tech, 2018 and 2021, and GSA Travel Award, 2020
- Dean's Honor fellowship, Rutgers, 2017
- Outstanding Student Awards (5% of 1000), 5 times, and Distinguished Leader of the Student Union, BUCT, 2014-2016