ANLU WEI

anlu.wei@manchester.ac.uk | Computational Chemistry

EDUCATION

University of Manchester | UK 09/2022 – Present

Ph.D. in Computational Chemistry

Tianjin University (985&211) | China 06/2019 – 06/2022

M.S. in Chemical Technology

GPA: 3.7/4.0 (87.6/100) Top 5/32

Khalifa University | UAE 01/2019 – 08/2019

Exchange Student in Molecular Simulation

China University of Petroleum (211) | China 09/2015 – 06/2019

B.E. in Chemical Engineering and Technology

GPA: 3.7/4.0 (88.2/100) Top 1/28

RESEARCH EXPERIENCE

University of Manchester | Advisor: Prof. Nikolas Kaltsoyannis 09/2022 – Present

Helium Migration in Zirconolite: A Density Functional Theory Study (J. Nuclear Materials, 2025)

Performed first-principles simulations (**DFT/VASP**) to map helium migration and diffusion in zirconolite across multiple vacancy types; quantified the influence of temperature and pressure on migration barriers, providing atomic-level insights that support zirconolite's application in HLW immobilization.

DFT Studies on Fructose Adsorption for Dehydration (Ongoing)

Developed and implemented DFT simulations (**VASP**) for fructose/HMF adsorption on sulfonated silica catalysts, creating a comprehensive conformer library and optimised slab models, which provided quantitative adsorption energy insights that guided experimental dehydration strategies.

Tianjin University | Advisor: Prof. Qingfeng Ge 06/2019 – 06/2022

CO_2 Methanation & Reverse Water Gas Shift on MoO_x-Ni Catalysts (J. Phys. Chem. C, 2022, Cover Article)

Conducted DFT simulations (**VASP**) to calculate stable adsorption structures, reaction energies, and energy barriers for CO_2 hydrogenation, constructing potential energy profiles to map reaction pathways. Performed Python-based microkinetic modelling to quantify pressure-dependent intermediate coverages and CH_4 selectivity.

Surface Modification in CO_2 Reduction Catalysis (J. CO_2 Utilization, 2021)

Designed and executed DFT simulations (**VASP**) to elucidate CO_2 adsorption behaviour on catalyst surfaces, integrating surface energetics, charge density mapping, and electronic state analysis to uncover the active sites and pathways relevant to catalytic performance.

Khalifa University | Advisor: Prof. Lourdes F. Vega 01/2019 – 08/2019

Amine Functionalization of MOFs for Enhanced CO_2 Capture (Front. Chem., 2021)

Screened the synthetized and hypothetical materials, including different degrees of functionalization, to identify key features of CO_2 adsorbent materials for gas flue applications. Performed **GCMC** molecular simulations (**LAMMPS**) to evaluate six amine models of different chain lengths and degrees of substitution in terms of adsorption isotherms, selectivity, cyclic working capacity, and regenerability.

Chinese Academy of Sciences| Advisor: Prof. Ning Wang, 06/2018 – 08/2018

Research on Graphyne Materials for Sodium-ion Battery Applications

Designed graphyne precursor molecules for electrochemical energy storage, optimizing electrode material performance. Separated alkyne-containing small molecules, ensuring high material purity and structural integrity. Assembled and tested alkali metal batteries to evaluate their energy storage capacity and cycling stability.

PUBLICATIONS

- **Wei, A**.; Kaltsoyannis, N. *Helium Migration in Zirconolite: A Density Functional Theory Investigation*, J. Nucl. Mater., 2025.
- **Wei, A**. et al. *Theoretical Insight into Tuning CO_2 Methanation and Reverse Water Gas Shift Reactions on MoO_x-modified Ni Catalysts*, J. Phys. Chem. C, 2022. (**Cover Article**)
- Zhang, R.; **Wei, A**. et al. *Tuning Reverse Water Gas Shift and Methanation Reactions during CO_2 Reduction on Ni Catalysts via Surface Modification by MoO_x*, J. CO_2 Utilization, 2021.
- Bahamon, D.; **Wei, A**. et al. *Effect of Amine Functionalization of MOF Adsorbents for Enhanced CO_2 Capture and Separation: A Molecular Simulation Study*, Front. Chem., 2021.

TEACHING EXPERIENCE

University of Manchester | Teaching Assistant 09/2023 – 06/2025

CHEM10600 - Python Exercise

Designed and implemented a systematic **Python** programming curriculum to teach fundamental coding principles for chemical problem-solving to undergraduates.

CHEM10600 - Gaussian Lab Training

Instructed undergraduates on quantum chemistry calculations using **Gaussian** and GaussView, covering Hartree-Fock methods, geometry optimizations, and analysis of molecular properties.

CONFERENCE PARTICIPATION

- 2025 30th Rare Earth Research Conference (RERC30) | Poster | Chicago, USA
- 2024 30th Materials Chemistry Consortium (MCC) Annual Meeting | Poster | Daresbury, UK
- 2024 11th International Conference on f Elements (ICFE11) | Poster | Strasbourg, France
- 2023 29th Materials Chemistry Consortium (MCC) Annual Meeting | Poster | Daresbury, UK

HONORS

- 2020 First-Class Scholarship, Tianjin University
- 2019 Special Excellent Scholarship, Tianjin University
- 2017 National Encouragement Scholarship (GPA top 5%), Ministry of Education
- 2017 Science and Technology Innovation scholarship, China University of Petroleum
- 2017 Prize for Excellence of Chemical Safety Design Competition, Ministry of Education
- 2016 The First Prize Scholarship (GPA top 3%), China University of Petroleum
- 2016 Outstanding Student, China University of Petroleum

SKILLS

- Computational Chemistry: *First-principles simulations (DFT: VASP, Gaussian, QE, CASTEP), MD (LAMMPS), GCMC, surface adsorption & reaction modelling, NEB/CI-NEB, charge analysis, electronic structure calculations.*
- Programming: *C++, Python, MATLAB*
- Languages: *IELTS 7.0*