

MIN Boya

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EDUCATION

Xi'an Jiaotong University (C9)

Master of Power engineering & Engineering Thermophysics

Xi'an, China

2019.9 - 2022.6

- **Supervisor:** Prof. GUO, Liejin & Prof. LIU, Maochang
- **Cumulative GPA:** 3.63/4.0
- **Thesis Title:** Synthesis of Multielemental Transition Metal Chalcogenides for Electrocatalytic Water Splitting

Southeast University (Project 985)

Bachelor of Chemical Engineering & Technology

Nanjing, China

2015.9 - 2019.9

- **Supervisor:** Prof. ZHOU, Jiancheng
- **Cumulative GPA:** 3.74/4.0, **Ranking:** 3/26
- **Thesis Title:** Synthesis and Mechanistic Study of Magnesium-Doped g-C₃N₄ for Enhanced Photocatalytic CO₂ Reduction

WORK EXPERIENCE

BYD Auto, Institute of Advanced Technology

Senior Battery Management System Engineer

Xi'an, China

2022.7 - Present

City University of Hong Kong Shenzhen Research Institute

Research Assistant (Part Time, Supervisor: Dr. Luoxiao YANG, School of Data Science)

Shenzhen, China

2024.7 - Present

RESEARCH INTERESTS

- Ai4Science, Deep learning, Electrocatalysis for water splitting, Photocatalytic CO₂ reduction, Advanced nanomaterials for catalysis
- Battery management system

RESEARCH PAPERS

1. **Min B.**, Yang L. and Zhang Z. M-MOFormer: Multi-Modal Transformer Framework for Metal-Organic Framework Property Prediction. *Thirty-Nine AAAI Conference on Artificial Intelligence (AAAI 2025, Workshop on AI to Accelerate Science and Engineering)*
2. **Min B.**[†], Wu W.[†], Li H., et al. NiFe-LDH coated NiSe/Ni foam as a bifunctional electrocatalyst for overall water splitting. *Reaction Chemistry & Engineering*, 2023, 8(7): 1711-1718.
3. Xue F., Guo X., **Min B.**, et al. Unconventional high-index facet of iridium boosts oxygen evolution reaction: how the facet matters. *ACS Catalysis*, 2021, 11(13): 8239-8246.
4. Wu W, Peng L, **Min B.**, et al. Activated overall water splitting over a Ni-Fe layered double hydroxide electrocatalyst by V doping and sulfuration. *Applications in Energy and Combustion Science*, 2023, 14: 100148.
5. Liu M, Chen G, **Min B.**, et al. Photocatalytic co2 reduction[J]. *Solar-to-Chemical Conversion: Photocatalytic and Photoelectrochemical Processes*, 2021: 243-267.

RESEARCH EXPERIENCE

1. Multi-Modal Transformer Framework for Metal-Organic Framework Property Prediction

2024.01 - 2024.11

- Developed M-MOFormer, a novel multi-modal transformer framework that integrates SMILES representations and automatically generated 2D structural diagrams through a self-developed openchemlib-MMOF package, significantly advancing the field of structure-agnostic MOF property prediction.
- Designed and implemented a dual-pathway transformer architecture featuring cross-modal attention mechanisms to effectively combine structural information from both textual and visual modalities, achieving superior prediction accuracy compared to existing structure-agnostic approaches while maintaining computational efficiency.

- Open-sourced a comprehensive multi-modal MOF prediction dataset and validated the framework's effectiveness through extensive experiments on two public datasets (QMOF and hMOF), demonstrating 7-11% improved prediction accuracy over state-of-the-art baselines while providing interpretable insights into structure-property relationships.

2. Synthesis of Multielemental Transition Metal Chalcogenides for Electrocatalytic Water Splitting

2021.04 - 2022.06

- **2.1 Synthesis and Electrocatalytic Performance of Ternary Transition Metal Sulfide NiFeV-S/NF**
 - * Developed a ternary transition metal sulfide NiFeV-S/NF catalyst via a two-step hydrothermal synthesis method to address the limitations of NiFe-LDH catalysts.
 - * Demonstrated superior electrocatalytic activity with overpotentials of 211 mV and 127 mV for OER and HER respectively, at a current density of 10 mA cm⁻² in 1 M KOH.
 - * Fabricated a NiFeV-S/NF//NiFeV-S/NF electrolyzer for overall water splitting, demonstrating outstanding performance with a low cell voltage of 1.573 V at 10 mA cm⁻².
- **2.2 Synthesis and Electrocatalytic Performance of NiSe@NiFe-LDH/NF Heterojunction Catalyst**
 - * Conceptualized and fabricated a novel core-shell heterostructured bifunctional electrocatalyst (NiSe@NiFe-LDH/NF), combining the high conductivity of NiSe with the catalytic activity of NiFe-LDH.
 - * Achieved exceptional electrocatalytic activity in alkaline conditions, used as both cathode and anode for electrocatalytic water splitting requiring only 1.560 V to deliver a current density of 10 mA cm⁻², surpassing the performance of previous catalysts.
 - * Conducted long-term stability tests to verify the durability enhancements provided by the core-shell architecture, contributing to the design of efficient and stable non-noble metal bifunctional catalysts.

3. Rational Design of Co-Cu/TiO₂ Photocatalyst for Efficient CO₂ Conversion via MOF-Templated Synthesis

2017.10 - 2019.03

- Developed a MOF-templated synthesis strategy using MIL-125(Ti) to fabricate hierarchically porous Co-Cu co-doped TiO₂ photocatalyst with precisely controlled surface composition and morphology.
- Elucidated the synergistic effect of Cu and Co dopants on charge carrier dynamics: Cu facilitates efficient photogenerated electron capture and separation, while Co acts as a hole trap and promotes H⁺ intermediate formation, enhancing C2+ product selectivity.
- Demonstrated superior photocatalytic performance in CO₂ reduction with H₂O, achieving high selectivity towards value-added C1-C3 products (CO, CH₄, C₂H₆, and C₃H₈) under simulated solar irradiation.

AWARD

- First Prize, Eastern China Region, 2nd National Undergraduate Chemical Engineering Experiment Competition
- President's Scholarship, Southeast University (Top 1%)
- Dalian Institute of Chemical Physics Scholarship (Top 5%)
- Jiangsu Electric Power Scholarship (Top 5%)
- Special Academic Scholarship, Xi'an Jiaotong University (Top 10%)

ENGLISH & GRE TESTS

- **GRE General Test:** Quantitative: 170 Verbal: 160 Analytical Writing: 4.0, Test Date: September 9, 2024
- **IELTS:** 6.0, 2023

Skill

- **Proficient in operation and data analysis:** TEM, SEM, XRD, FTIR & UV-vis spectroscopy
- **Familiar with basic functions:** Aspen Plus, 3D MAX, ChemDraw, Origin
- **LLM Tools:** GPT-4, Claude 3.5, Research productivity enhancement, Coding assistance