

Xu (Melissa) HUANG

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EDUCATION

Shanghai Jiao Tong University (SJTU)

B.E. in Chemical Engineering and Technology

Shanghai, China

Sep. 2019 – Jun. 2023 (expected)

- Major GPA: 4.00 / 4.00 (Ranking: 1 / 24)

PUBLICATION

- Yang, L., Ding, Y., **Huang, X.**, Gao, Y., Hua, C., He, Y.*, Economics of Processes Involving CO₂ in Circular Economy, *Circular Economy Processes for CO₂ Capture and Utilization*, Elsevier, 2022, **Invited book chapter** (in press)

RESEARCH EXPERIENCES

Computer-Aided Synthesis Planning | *Independent Research*

Jul. 2022 – Present

Advisor: Prof. Yiming Mo, Mo Research Lab, Zhejiang University (ZJU)

- Constructed the data-driven model of retrosynthesis in Python, leveraging molecular similarity to propose and rank one-step retrosynthetic disconnections based on analogy to precedent reactions;
- Achieved the top-50 exact matching accuracy of 80.86% in 5000 test reactions, using 45000 reactions from the United States patent literature as a knowledge base;
- Exploring automated methods for extracting synthetic reactions of energetic materials from chemical literature as the training data set to improve the model's predictive accuracy in energetic materials synthesis.

Optimization of an Automatic Platform for Microflow Synthesis | *Team Leader*

Oct. 2021 – Present

Advisor: Prof. Yuanhai Su, Continuous-Flow Reactor Technology Research Group, SJTU

- Operated the automatic platform for the photoisomerization of norbornadiene to quadricyclane;
- Screened and optimized the structures of the photomicroreactor, increasing the space-time yield of the organic synthesis to at least 40 times higher than some previously reported ones;
- Optimized the chromatographic temperature to correct reaction yield from normally reported 93% to nearly 100%.

Magnesium-Air Battery Based on Dual-Layer Gel Electrolyte | *Independent Research*

Sep. 2021 – Jun. 2022

Advisor: Prof. Yanna Nuli, Electrochemistry and Energy Technology Institute, SJTU

- Synthesized and spread the 200 μm thick polyethylene oxide and polyacrylamide thin films over the Mg sheet;
- Assembled Mg-air battery with the dual-layer gel electrolyte of the sandwich type and the cable type;
- Enabled the battery to discharge stably for over 60h with a low voltage and improved Mg utilization by replacing the dense passive magnesium hydroxide layer with the loose needle-like discharge product.

Investigation on Covalent Modification of Black Phosphorus | *Team Member*

Oct. 2020 – Oct. 2021

Advisor: Prof. Gang Liu, Brain-Inspired and Smart Bionic Device Lab, SJTU

- Synthesized diazonium tetrafluoroborate of triphenylamine (DTPA) by sequential nitration, amination, and diazotization of triphenylamine (TPA);
- Prepared TPA-modified black phosphorus nanosheets (BPNSs-TPA) by the nucleophilic addition reaction;
- Doped BPNSs-TPA into polyvinyl pyrrolidone to construct the resistive random access memory (RRAM), exhibiting the nonvolatile rewritable performance with excellent endurance over 150 switching cycles.

SELECTED AWARDS & HONORS

- China National Scholarship (**top 0.2%, the highest honor for university students in China**, 2021, 2022),
- China National Scholarship for Encouragement (**top 3%, the highest honor for impoverished students**, 2020),
- Excellent Leader (**top 0.3%**, 2022), Xipu Reading Scholarship (2022), Excellent Student (**top 3%**, 2020),
- Honor Cadre (**top 0.3%**, 2021), Honor Student (**top 3%**, 2020)

EXTRA-CURRICULAR PROJECTS

Osaka University Student Exchange Virtual Program

Oct. 2022 – Feb. 2023 (expected)

- Learning bioinformatics, algorithms and theory of computing, high-performance computing, software analysis, project management, information networks, information security, and so on.

ShanghaiTech University Material Science Summer School

Aug. 2022 – Aug. 2022

- Learned characterization techniques, principles, and recent applications of emerging photonics technologies.

National College Student Chemical Engineering Design Competition

Mar. 2022 – Jun. 2022

- Designed a factory that produces 1,4-Butanediol, including the projects of Aspen simulation for reaction and separation procedures, the heat exchange network (HEN), the Piping and Instrumentation Diagram (P&ID), the economic evaluation, and the plant design AutoCAD drawing;
- Won the third prize in the Shanghai division (**China's highest-level competition in chemical engineering**).