Xu (Melissa) HUANG

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EDUCATION

Shanghai Jiao Tong University (SJTU) Shanghai, China
B.E. in Chemical Engineering and Technology 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 CO_2 in Circular Economy, *Circular Economy Processes for CO_2 Capture and Utilization*, *Elsevier*, 2022, **Invited book chapter** (in press)

RESEARCH EXPERIENCES

Computer-Aided Retrosynthesis 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.

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 coated the polyethylene oxide and polyacrylamide thin films across the surface of 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.

Optimization of an Automatic Platform for Microflow Synthesis | *Team Leader* Nov. 2021 – Mar. 2022
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%.

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), Xinpu 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**).