Xu (Melissa) HUANG

+86 13982026448 | meli.ssa@sjtu.edu.cn | xuhuang.netlify.app

EDUCATION

Shanghai Jiao Tong University (SJTU) Shanghai, China
B.E. in Chemical Engineering and Technology Sep. 2019 – Jun. 2023 (expected)

- Overall Ranking: 1 / 24 (Major GPA: 4.00 / 4.00)
- Computer Simulation In Chemical Engineering Process (100), Chemical Process Control (97), Chemical Technology (97), Thermodynamics in Chemical Engineering (95), Chemical Engineering (94), Elements of Chemical Reaction Engineering (94)

Osaka University Osaka, Japan
Student Exchange Program Oct. 2022 – Feb.2023 (expected)

- Information science, including bioinformatics, algorithms and theory of computing, high-performance computing, software analysis, information networks, information security

ShanghaiTech University Shanghai, China
Materials Science Summer School Aug. 2022

- Characterization techniques and applications of emerging photonics technologies

RESEARCH EXPERIENCE

Computer-Assisted Synthesis Planning Jul. 2022 – Present
Advisor: Prof. Yiming Mo, Zhejiang University (ZJU) | *Independent Research*

- Constructed the data-driven model of retrosynthesis in Python using the open-source RDChiral wrapper for RDKit, leveraging molecular similarity to propose and rank one-step retrosynthetic disconnections based on analogy to precedent reactions;
- Achieved the top-50 accuracy of 80.84% in 5000 test reactions, using 45000 reactions from patents as a knowledge base, which could help to create more intelligent synthetic platforms;
- Took the initiative to collect and process 16280 reactions as the first open-access datasets of specialty chemicals reactions, improving the model's top-50 accuracy from 0.00% to 5.06% in proposing candidate precursors for specialty chemicals.

Performance Boost for Mg-Air Batteries Using Novel Electrolytes Sep. 2021 – Present
Advisor: Prof. Yanna NuLi, SJTU | *Independent Research*

- Synthesized and spread the 200 μm thick polyethylene oxide and polyacrylamide thin films over the Mg sheet as the dual-layer gel electrolyte in Mg-air batteries;
- Enabled the batteries to discharge for over 60h with a stable voltage and replaced the dense passive $Mg(OH)_2$ layer with the loose discharge product $Mg_2Cl(OH)_3$, which presented an innovative thinking for overcoming the biggest bottleneck in Mg-air batteries concerning the high corrosion rate and low utilization of Mg anode;
- Formulated the mechanism for the corrosion of Mg to select the optimal electrolyte additive, the 2,6-dihydroxybenzoate, for aqueous Mg-air batteries, with the average evolved hydrogen amount dropped by 37.5% compared to the blank ones.

Optimization of an Automatic Platform for Microflow Synthesis Oct. 2021 – Nov. 2022
Advisor: Prof. Yuanhai Su, SJTU | *Team Leader*

- Operated the automatic platform for the synthesis from norbornadiene to quadricyclane which could be used as an excellent high-energy fuel;
- Screened and optimized the reactors by analyzing the relationship between the reaction rate

constant and the structures of the photomicroreactor, increasing the space-time yield of the organic synthesis to at least 40 times higher than previously reported ones;
- Optimized the chromatographic temperature to correct reaction yield from normally reported 93% in literature to nearly 100%.

Investigation on the covalent modification of Black Phosphorus Oct. 2020 – Oct. 2021
Advisor: Prof. Gang Liu, SJTU | *Team Member*

- Designed and 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, which exhibited a huge improvement of 5 times in anti-oxidation capacity;
- Doped BPNSs-TPA into polyvinyl pyrrolidone to construct the resistive random access memory, exhibiting the nonvolatile rewritable performance with excellent endurance over 150 switching cycles, which provided a new idea for building high-performance computers.

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)

SELECTED AWARDS & HONORS

- National Scholarship (top 0.2%, highest nationwide honor for merit students) 2021, 2022
- National Endeavor Scholarship (highest honor for need-based merit students) 2020
- Xinpu Reading Scholarship (26 / 40000+ for outstanding reading habits) 2022
- 3rd prize in National ChemE Design Competition (highest-level competition) 2022
- Excellent Leader (top 0.3% at SJTU) 2022
- Merit Cadre (top 0.3% at SJTU) 2021
- Excellent Member (top 3% at SJTU) 2020
- Merit Student (top 3% at SJTU) 2020

LEADERSHIP & VOLUNTEERING

Leadership in Student Organizations

- Carried on a crucial reform in the organizational structure and handled general affairs, as president of the Students Commission of SJTU Library, which has over 500 students;
- Planned a series of school activities, as a Student Union officer;
- Organized long-term voluntary work in traffic control, as captain of Security Department.

Volunteering in Social Services

- Initiated the university-wide "Book Bank" plan to donate books to children in poor mountainous areas as well as foster an excellent reading atmosphere at SJTU;
- Devoted over 700h to voluntary work, for instance, volunteering in Shanghai Marathon;
- Participated in charity work, for instance, by being a team leader and interviewer of the Green Grid Charity Group, which is reported and highly praised by China Central Television for its contribution to the prevention and control of desertification.

SKILLS & INTERESTS

- **Software Skills**: Python, C/C++, MATLAB, Aspen Plus, AutoCAD, ChemDraw, LaTeX
- **Research Interests**: autonomous discovery, machine learning, chemical synthesis, materials and molecular design, laboratory automation, molecular dynamics, sustainable energy