

Jingyi Liu

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Academic Qualifications

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| Erasmus Mundus Master of Theoretical Chemistry and Computational Modelling
<i>Katholieke Universiteit Leuven</i> | 09/2022-07/2024
<i>Belgium</i> |
| <ul style="list-style-type: none">• Graduate with <i>Cum Laude</i>• Thesis: QM/MM calculations on the photochemical dynamics of LSSmOrange• Key courses: Quantum chemistry, Statistical Mechanics, Chemistry in Motion, Group Theory, DFT | |
| Erasmus Exchange Program
<i>University of Barcelona, University of Valencia, and Autonomous University of Madrid</i> | 09/2023-02/2024
<i>Spain</i> |
| <ul style="list-style-type: none">• Completed coursework in Machine Learning, QSAR, Simulations of Materials, Advanced Computational Techniques, etc. as part of the degree | |
| Bachelor of Science in Applied Chemistry
<i>Tongji University</i> | 09/2018-02/2022
<i>China</i> |
| <ul style="list-style-type: none">• graduate with a total GPA of 86.88/100• Thesis: Structure-property Modeling for Polyimide via Machine Learning• Key courses: Organic, Inorganic, Analytical, and Physical Chemistry, Laboratory, Advanced Mathematics, Linear Algebra | |

Previous Research Work

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| Study of isomerization step of [P,O]-chelated nickel catalysts
<i>Supervisor: Prof. Xinglong Zhang</i> | 10/2024-present
<i>Chinese University of Hong Kong, China</i> |
| <ul style="list-style-type: none">• Assisted in the revision of a research article on the isomerization processes involved in Nickel-catalyzed copolymerization of ethylene with polar monomers.• Contributed to refining the study's interpretation of DFT results, focusing on the mechanism and influence of auxiliary groups on catalyst performance. | |
| QM/MM calculations on the photochemical dynamics of LSSmOrange
<i>Master's Thesis – Supervisors: Prof. Daniel Escudero, Prof. Jeremy Harvey</i> | 09/2023-06/2024
<i>KU Leuven, Belgium</i> |
| <ul style="list-style-type: none">• Explored new flavors of electronic structure methods, photo-physics and excited-state dynamics to calculate the excited state dynamics of LSSmOrange fluorescence protein by employing semi-empirical methods and a multi-scale technique.• Investigated surface-hopping behaviour of excited state proton transfer process of LSSmOrange. | |
| Solving 1D Schrödinger Equation for Vibrational Energy Numerically
<i>Research Internship – Promotor: Prof. Jérôme Loreau</i> | 02/2023-06/2023
<i>KU Leuven, Belgium</i> |
| <ul style="list-style-type: none">• Employed the discretization method of wavefunction and mathematical transformation to code for a program to solve the Schrödinger equation for the bending mode of triatomic molecules based on the Hamiltonian proposed by Carter and Handy | |
| Structure-property Modeling for Polyimide via Machine Learning
<i>Bachelor's Thesis</i> | 12/2021-06/2022
<i>Tongji University, China</i> |
| <ul style="list-style-type: none">• Adopted machine learning method to indicate the significance of structures for rapid prediction of glass-transition temperature of polyimides.• Adapted 2D structural formulas into SMILES format and used online open libraries including RDkit to calculate the values of molecular descriptors• Explored the applications of linear regression, random forest and artificial neural network in QSAR modelling. | |
| MobiDraw- An Intelligent Identification Mobile Terminal Chemical Mapping App
<i>Chinese National College Student Innovation and Entrepreneurship Training Project</i> | 03/2021-03/2022
<i>Tongji University, China</i> |
| <ul style="list-style-type: none">• Worked in a five-person team to program a Chemical Mapping App which can convert handwriting chemical formula into codes. | |
| Synthesis of Polimide Ionogel for Memory Materials and Strain Sensor
<i>National College Students Chemical Experiment Innovation Design Competition project</i> | 03/2020-09/2021
<i>Tongji University, China</i> |

- Lead a 3-person team to synthesized a polyimide ionogel maintaining both excellent mechanical and magnetic properties.
- Proposed a new method to embed nanoparticle ferroferric oxide into a new polymer framework.

Green Synthesis of Virginiamycin

03/2020-03/2021

College Students Innovation Training Program

Tongji University, China

- Worked in a 2-person team on low-cost, high selectivity synthesis of Virginiamycin via Wittig Reaction.

Previous Academic Position

Teaching Assistant

09/2021-02/2022

Analytical Chemistry Laboratory, Tongji University

China

- Assisted in preparing and grading assignments, quizzes, and exams, providing timely feedback to students.
- Collaborated with the professor to design and update course materials, including lab experiments and lecture slides.

Present Academic Position

Incoming PhD student at the Department of Chemistry, Chinese University of Hong Kong

Supervisor: Prof. Xinglong Zhang

Publication

- Tan, J., Liu, J., and Zhang, X. (2024). Unravelling the mechanism and influence of auxiliary ligands on the isomerization of neutral [P,O]-chelated nickel complexes for olefin polymerization. *Submitted*.