Contact Information

Name: Zhao Weiren
Phone (WeChat): 13980339144
Email: 32227015@mail.dlut.edu.cn
Personal Page:Zhao Weiren
Supervisor's Profile: Li Yang

Statement of Purpose

Zhao Weiren

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Hello, this is Zhao Weiren. I am currently pursuing my Master's degree under the supervision of Associate Professor Li Yang at Dalian University of Technology, scheduled to graduate in 2025. Our research group focuses on utilizing machine learning algorithms for catalyst design and reaction prediction, constructing innovative GNN models to accomplish chemistry-related research tasks.

1 Personal and academic background:

Under the guidance of Professor Li Yang (Research areas: computational organic chemistry, reaction mechanism studies, catalyst design and reaction prediction using machine learning), I have delved into the application of machine learning in the field of chemistry and accumulated extensive experimental and theoretical knowledge. During my master's program, not only have I mastered English (with a **CET-6** score of **550** and preparing for the IELTS exam), but I also proficiently use Python along with its scientific plotting and machine learning libraries (such as **PyTorch**, **Sklearn**, **RDKit**, **PyG** and **So on**) for data analysis and model construction. Additionally, I am familiar with computational chemistry software (like **Gaussian**, **Multiwfn**, **VMD**) and the writing of Windows batch scripts (**Bat**) and **TCL** commands. I know how to utilize Google's machine learning cloud resources such as **Colab** for model training, have participated in basic and intermediate level Vasp software usage training, and possess a foundational understanding of **Vasp**. These skills provide strong technical support for my research.

2 Research achievements and group status:

Although our research group's work in the field of machine learning is still in its early stages, through extensive literature review and in-depth study, I independently completed a machine learning research project titled "Predicting the Yield of Pd-catalyzed Buchwald-Hartwig Amination using Machine Learning with Extended Molecular Fingerprints and Selected Physical Parameters" which has been accepted for publication in an SCI journal. In this work, I was responsible for model design, experiment execution, data analysis, paper writing, and addressing reviewer comments. This paper is the result of joint efforts with my associate professor Li Yang, marking the first step of our group in the field of machine learning.

3 Motivation for Joining Your Group:

Since beginning my master's program, I've been captivated by the fusion of machine learning with materials chemistry—a field where chemical insight meets data science, opening new horizons for material innovation. Over the past few years, I've built a strong foundation in this area, honing both practical and computational skills with a commitment

to scientific excellence. My expertise aligns well with your team's focus, as evidenced by my master's research, which paralleled your lab's interests. I'm eager to combine my skills with your team's knowledge to propel our shared passion for this dynamic field forward. I believe I can integrate smoothly into your group, contributing fresh perspectives and energy. Pursuing a PhD under your guidance is my goal, aiming to achieve significant academic milestones. I look forward to the opportunity to collaborate, explore scientific frontiers, and help shape the future together.

4 Ongoing Research Projects:

- **Introduction Research Projects:**
  - *Project One:* **Innovative GNN Model Input Representation.**
    - **Objective:** Enhance the Graph Neural Network (GNN) model's understanding of intermolecular interactions through innovative input data representation, improving reaction interpretation to guide chemical experiments.
    - **Progress:** Preliminary results have been achieved; the project is expected to complete relevant tasks in three months and begin journal submission.
  - *Project Two:* **Multimodal Model for HTE Data Analysis.**
    - **Collaboration:** Undertaken with an undergraduate student, developing a multimodal model utilizing GNN to analyze classical High-Throughput Experimentation (HTE) data for reaction interpretation and experimental guidance.
    - **Status:** Experimental content is completed, currently in the process of paper writing for submission.
  - *Future Plan:* **Integration of ML Models and Experiments for Material Design.**
    - **Vision:** Combine ML models, especially GNNs, with pre-trained and generative models to design chemistry-related materials guided by properties and functions.
    - **Strategy:** Focus on studying and innovating bipartite graphs to improve GNN learning efficiency for more comprehensive and accurate material information capture, followed by experiment verification.

5 Current results:

- Zhao, W.R., & Li, Y. (in press). Predicting the Yield of Pd-Catalyzed Buchwald-Hartwig Amination Using Machine Learning with Extended Molecular Fingerprints and Selected Physical Parameters. ChemistrySelect. (Accepted for Publication)