

Haoming Su

Email: suhaoming@stu.scu.edu.cn | Phone: (+86)-15023765900

EDUCATION

Sichuan University

2020.09-2024.06

Bachelor of Chemistry

Relevant Courses: Chemoinformatics, Analytical Chemistry, Organic chemistry, Inorganic Chemistry, Physical Chemistry, Biochemistry, Molecular and Supramolecular Photochemistry, Nuclear Energy and Reprocess Technology for Nuclear Fuel, Nuclear Technology and Applications, Organic Stereochemistry, Mechanism of Organic Reaction, Synthetic Chemistry, Computational Thinking and Computer

GPA:3.68

Ranking:16/189

IELTS:7.5 :L 8.5 R 8.5 W 6.5 S 5.5

GRE: preparing

RESEARCH EXPERIENCE

Deep Learning Based Prediction of PLQY for OLED Materials

2022.09-2023.09

- Used deep learning methods to build a prediction model for PLQY of OLED materials, thus achieving fast and accurate PLQY prediction and aiding OLED material design.
- Collected and cleaned a total of about 14,000 fluorescent molecules data from open source databases such as chemfluor, deep4chem, etc.
- Introduced K-fold cross-validation, regularization, and other methods to address the problem of poor accuracy of ordinary machine learning models due to noisy data sets, thus enhancing model generalization and improving prediction accuracy.
- Adopted Bayesian method for hyperparameter search and optimized the model structure.
- Shortened the time-consuming TD-DFT calculation (elapsed time = hours) to an immediate structure-property prediction with no significant difference in accuracy, which can reduce the design time of the material.

Simulation and Application Studies in the Design of New Small Organic Molecules in Perovskite Solar Cells Based on Quantum Calculations and Artificial Intelligence

2022.09-2023.09

- Designed HTL layer molecules for novel low band gap perovskite solar cells.
- Took charge of the design of the molecules and used computational chemistry software Gaussian/multiwfn and artificial intelligence for property calculation, prediction and synthesis.
- Prepared the HTL layer by spin-coating, the chalcogenide layer by one-step antisolvent method, and the ETL layer and top electrode by vacuum vapor deposition. The resulting devices have good structural hole extraction and transport ability, smooth surface of the chalcogenide films, and good photovoltaic performance of the devices.

The Recycling of Biodegradable Polymer Products

2021.09-2022.07

- Conducted a literature review and completed relevant experimental manipulations to recover PLA through studying lewis acid catalysts.

PUBLICATIONS

- [1] Guo, J., Sun, M., Zhao, X., Shi, C., Su, H., Guo, Y., & Pu, X. (2023). General Graph Neural Network-based model to accurately predict cocrystal density and insight from data quality and feature representation. Journal of Chemical Information and Modeling, 63(4), 1143–1156. <https://doi.org/10.1021/acs.jcim.2c01538>

SKILLS

Equipment: Schlenk Line, Column Chromatography, HPLC, FT-IR, UV-Vis, TEM, SEM, AFM, Ramam, XRD, TGA, DSC

Software: Origin, ChemDraw, Endnote, Mestrenova, Gaussian, Multiwfn, and basic skills and interests of python programming and neural network