Houyou Lei

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EDUCATION

Shanxi University Taiyuan, Shanxi

- **Dual Degree:** B.Eng. in Applied Chemistry & B.Sc. in Biology Sept 2020 - Jun 2024
- **Overall GPA:** 3.29/4.0 (Last Two Years: 3.76/4.0)

PUBLICATIONS

- R. Xu†, Y. Jiang†, **H. Lei**†, F. Liu*, K. Liu, L. Feng, G. Ran, W. Zhang, C. Zhong*, X. Zhu*. 'Enhancing the formation of delocalized singlet excitons via asymmetric fluorination of nonfullerene acceptors for efficient organic solar cells.' Science Advances. Under Review. († denotes equally contributing authors)

RESEARCH EXPERIENCE

Full-time Research Assistant Jun 2024 - Present

Theoretical Analysis of the Effect of Asymmetric Terminal Fluorination Strategies on Dimer Stacking

Institute of Chemistry, Chinese Academy of Sciences

Advisor: Prof. Feng Liu, Assoc Prof. Cheng Zhong

- Extracted representative dimer configurations from the simulation trajectories using VMD, after performing molecular dynamics simulations on Z-series acceptors with GROMACS.
- Explored the stacking differences induced by asymmetric fluorination in Z-series molecules by quantifying the number of π-π interactions between donor and acceptor segments of Z-series molecules in acceptor film using a Python script with MDAnalysis.
- Calculated the interaction energies with BSSE correction by Gaussian and explored the interaction differences of various terminal stackings.
- Determined the exciton recombination and dissociation pathways by calculating the distribution of electron-hole pairs on the donor and acceptor.
- Calculated the free volume ratio(FVR) for three molecular systems based on the simulation results of GROMACS.

Research Assistant Sept 2023 - Sept 2024

Research on the Excited State Properties and Energy States of Brominated Asymmetric Receptor Dimers

Shanxi University

Advisor: Assoc Prof. Hu Shi, Assoc Prof. Cheng Zhong

- Optimized w parameter of the long-range corrected density functional and calculated the LE state and CT state energies of the synthesized brominated asymmetric acceptor molecules to reflect the non-radiative energy losses.
- Calculated the ground state, S1 state, and T1 state energy levels, as well as the electron-hole distribution and charge density difference for two brominated asymmetric non-fullerene acceptor molecules, to investigate the effect of bromine substitution on the excited states.
- Ascertained the contribution of Br to the HOMO/LUMO and calculated the spin-orbit coupling (SOC) matrix of the two molecules to evaluate the possibility of intersystem crossing (ISC).

Research Assistant Jul 2021 - Sept 2023

Synthesis and Photovoltaic Performance Analysis of Brominated Asymmetric Non-Fullerene Acceptor Materials and PDI Derivatives
Shanxi University
Advisor: Prof. Feng Liu

- Designed the synthesis route of brominated asymmetric non-fullerene acceptor materials by SciFinder.
- Synthesized two types of brominated asymmetric non-fullerene acceptor materials.
- Identified the product structure by analyzing the 1D ^{1}H NMR spectrum with MestReNova.
- Characterized the electrochemical band gap of the two molecules via cyclic voltammetry and calculated the optical band gap from the UV-Vis absorption edge.
- Analyzing the GIWAXS spectra to explore the crystallographic orientation of acceptor films.
- Determined exciton dissociation time at the interface and diffusion time to the D/A interface by analyzing Femtosecond Transient Absorption Spectroscopy.

Research Assistant Nov 2020 - Jul 2021

Simulation of the Photoelectric Effect and Critical Analysis of Ternary Mixtures
Shanxi University
Advisor: Prof. Feng Liu

- Simulated the Shockley-Queisser Limit using Python with SciPy, NumPy, and Matplotlib.
- Calculated the critical concentration of ternary mixtures by writing a Python script with Sympy to solve the Flory-Huggins Equation.

PERSONAL PROJECT

- Constructing the STO-3G basis set for the hydrogen by obtaining contracted gaussian function(CGF) combination coefficients through fitting STOs.
- Writing an RHF program in Python using the PySCF libcint interface.

SKILLS

- **Programming:** Shell (bash), C, Python.
- **Computational Chemistry:** GROMACS, xtb, Gaussian, ORCA, PySCF, RDKit, Multiwfn, Packmol, VMD, MDAnalysis.
- **Synthesis:** ChemOffice, MestReNova, SciFinder.
- **Data Visualization:** Origin, Matplotlib.