Houyou Lei

Mobile:+(86)-18728451378 E-mail: leihouyou@alu.sxu.edu.cn
Personal website: LeiHoyo.github.io

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. Peer review completed, in revision based on major comments († 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 Acceptor 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

- Independently designed and synthesized two types of brominated asymmetric non-fullerene acceptor materials, achieving a power conversion efficiency (PCE) of 18.48% with J_{SC} of 25.16 mA cm^{-2} and V_{OC} of 0.94 V for one material, and a PCE of 17.11% with J_{SC} of 23.38 mA cm^{-2} and V_{OC} of 0.95 V for the other.
- Characterized the electrochemical band gap of the two molecules via cyclic voltammetry and calculated the optical band gap from the UV-Vis absorption spectrum.
- 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 for phase separation in ternary mixtures by writing a Python script with Sympy.

PERSONAL PROJECT

- Constructing the STO-3G basis set for the hydrogen by obtaining contracted gaussian function(CGF) combination coefficients through fitting STOs.
- Developed a Python program with libcint library to solve Restricted Hartree-Fock (RHF) equations for diatomic molecules via the self-consistent field (SCF) method.

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.
- **Scientific Writing**: LaTeX, Microsoft Word.