Houyou Lei

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EDUCATION

Shanxi University Taiyuan, Shanxi
- **Degree:** B.Eng. in Applied Chemistry 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. DOI: 10.1126/sciadv.adt6024 . († denotes equally contributing authors)

RESEARCH EXPERIENCE

Full-time Research Assistant Jun 2024 - Dec 2024

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

Institute of Chemistry, Chinese Academy of Sciences

Advisor: Prof. Feng Liu, 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 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 - Jun 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.
- Calculated the critical concentration for phase separation in ternary mixtures.

PERSONAL PROJECT

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

SKILLS

- **Computational Chemistry Software:** GROMACS, Gaussian, ORCA, VMD, MDAnalysis.
- **Synthesis Tools:** ChemOffice, MestReNova, SciFinder.
- **Data Visualization Software:** Origin, Matplotlib.
- **Scientific Writing**: Markdown, Microsoft Word.