

Lewen Wang

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Education

- **Sun Yat-sen University (Guangzhou)** **Sep.2020 – Jun.2022**
Master of Engineering in *Materials and Chemical Engineering*
- **Beijing University of Chemical Technology (Beijing)** **Sep.2016 – Jun.2020**
Bachelor of Engineering in *Polymer Materials and Engineering*

Main Research Experience

A Theoretical Design of Chiral Molecules through Conformational Lock.

May.2021 - Jun.2022

- **Abstract:**
 1. A new strategy was developed to create chiral organic small molecules for generating circularly polarized (CP) light.
 2. Chirality was introduced into molecules through a conformational lock, involving achiral light-emitting groups and alkyl chains.
 3. Simulations showed that the chirality can be tuned by extending the alkyl chains connected to the diketopyrrolopyrrole core.
 4. Chiroptical properties were validated both by simulations and experimental data.
- **Contribution:** Investigation, molecular simulation, coding, data processing & curation, article writing.

Machine Learning Predicts the Electronic Couplings in Organic Semiconductors.

Nov.2020 – May.2021

- **Abstract:**
 1. New intermolecular 3D descriptors were developed to predict electronic couplings in both crystalline and amorphous organic thin films.
 2. The developed descriptors outperformed the most advanced existing descriptors in terms of speed and accuracy.
 3. This advancement facilitates large-scale simulations, high-throughput calculations, and screening of organic semiconductors.
- **Contribution:** Investigation, molecular simulation, coding, data processing & curation.

Studying N-Type Organic Semiconductors Through Molecular Calculations.

- **Aldol Polymerization to Construct Half-Fused Semiconducting Polymers.** **Feb.2021 – Apr.2021**
- **Green Synthesis of Lactone-Based Conjugated Polymers for n-Type Organic Electrochemical Transistors.** **Jun.2021 – May.2022**
- **Donor Functionalization Tuning the N-Type Performance of Donor–Acceptor Copolymers for Aqueous-Based Electrochemical Devices.** **Oct.2021 – Jul.2022**
- **Highly Efficient Mixed Conduction in N-type Fused Small Molecule Semiconductors.** **Oct.2021 – Apr.2022**
- **Contribution:** Molecular simulation, data curation, formal analysis, technical guidance, article writing.

Fabrication of Skin Wound Healing Materials Based on Decellularized Tissue Scaffolds.

Nov.2018 – Jun.2019

- **Abstract:**
 1. This study focused on developing decellularized scaffold materials for wound dressings.
 2. We specifically examined the superior wound healing properties of pig small intestine matrices.

3. An oxygen-releasing hydrogel composite was synthesized by freeze-drying and grinding the matrix, combined with degradable oxygen-releasing microspheres and chitosan film.

4. This novel material provided enhanced mechanical strength, biocompatibility, and accelerated wound healing through oxygen release.

■ **Contribution:** Material preparation, literature review, animal experimentation, data curation.

Professional Skills

Experiment: Understand and familiar with experimental instruments for **materials preparation**, **testing** and **characterization**; have experience in **polymer physics**, **polymer chemistry** and **animal experiments**.

Molecular calculation: Proficient in molecular modeling, DFT calculation and visualization with **Gaussian**; understand molecular dynamics simulation with **Gromacs**; able to write various script for automating calculation procedures and handling computational data.

Programming: Proficient in **Python**, able to code with **C++**, used to working in **Linux**.

Machine learning: Have experience in constructing and training neural networks using **TensorFlow**; still learning **Pytorch**.

Language: Proficient in communication in English, Mandarin, and Cantonese; IELTS score of 7.0 (2021), CET6 score of 591.

Publications

- **Wang, L.**; He, T.; Liao, H.; Luo, Y.; Ou, W.; Yue, W.; Long, G.; Wei, X.; Zhou, Y. A Theoretical Design of Chiral Molecules through Conformational Lock towards Circularly Polarized Luminescence. *Photonics* 2022, 9(8), 532.
- Ma, J.#; Du, Z.#; Lei, Z.#; **Wang, L.**; Yu, Y.; Ye, X.; Ou, W.; Wei, X.; Ai, B.; Zhou, Y. Intermolecular 3D-MoRSE Descriptors for Fast and Accurate Prediction of Electronic Couplings in Organic Semiconductors. *J. Chem. Inf. Model.* 2023, 63, 16, 5089–5096.
- Sun, Y.; **Wang, L.**; Guselnikova, O.; Semyonov, O.; Fraser, J.; Zhou, Y.; López, N.; Ganin, A.Y. Revealing the activity of Co₃ Mo₃ N and Co₃ Mo₃ N_{0.5} as electrocatalysts for the hydrogen evolution reaction. *J. Mater. Chem. A*, 2022, 10, 855-861.
- Guo, Y.; Yang, X.; **Wang, L.**; Duan, J.; Zhou, Y.; Nielsen, C.B.; Yu, Y.; Yang, J.; Guo, Y.*; Li, Z.; Yue, W.*; Liu, Y.; McCulloch, I. Aldol Polymerization to Construct Half-Fused Semiconducting Polymers. *Macromolecules* 2021, 54, 22, 10312–10320.
- Wang, Y.; Zeglio, E.; **Wang, L.**; Cong, S.; Zhu, G.; Liao, H.; Duan, J.; Zhou, Y.; Li, Z.; Mawad, D.; Herland, A.; Xue, W.; McCulloch, I. Green Synthesis of Lactone-Based Conjugated Polymers for n-Type Organic Electrochemical Transistors. *Adv. Funct. Mater.* 2022, 32(1), 202111439.
- Cong, S.; Chen, J.; **Wang, L.**; Lan, L.; Wang, Y.; Dai, H.; Liao, H.; Zhou, Y.; Yu, Y.; Duan, J.; Li, Z.; McCulloch, I.; Xue, W. Donor Functionalization Tuning the N-Type Performance of Donor–Acceptor Copolymers for Aqueous-Based Electrochemical Devices. *Adv. Funct. Mater.* 2022, 32(18), 202201821.
- Chen, J.; Cong, S.; **Wang, L.**; Wang, Y.; Lan, L.; Chen, C.; Zhou, Y.; Li, Z.; McCulloch, I.; Yue, W. Backbone Coplanarity Manipulation via Hydrogen Bonding to Boost the n-Type Performance of Polymeric Mixed Conductors Operating in Aqueous Electrolyte. *Mater. Horiz.* 2023, 10(2), 607–618.
- Duan, J.; Zhu, G.; **Wang, L.**; Chen, J.; Cong, S.; Zhu, X.; Zhou, Y.; Li, Z.; McCulloch, I.; Xue, W. Highly Efficient Mixed Conduction in N-type Fused Small Molecule Semiconductors. *Adv. Funct. Mater.* 2022, 32(34), 2203937.
- Wang, X.; Cao, Y.; Peng, Y.; **Wang, L.**; Hou, W.; Zhou, Y.*; Shi, Y.; Huang, H.; Chen, Y.; Li, Y.* Concurrent and Mechanochemical Activation of Two Distinct and Latent Fluorophores via Retro-Diels–Alder Reaction of an Anthracene–Aminomaleimide Adduct. *ACS Macro Lett.* 2022, 11, 310–316.

Work Experience

■ **TP-LINK (Shenzhen)**

Sep.2022 – Apr.2024

System Test Engineer