Cheng-Han Li

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Education

Texas A&M University (TAMU) — *College Station, TX*

Ph.D. Candidate in Chemistry (GPA: 4.0/4.0) — *Sept 2019 - 2024 (expected defense)*

Advisor: Daniel P. Tabor

National Taiwan University (NTU) — *Taipei, Taiwan*

B.S. in Chemistry (GPA: 3.9/4.3) — *Sept 2015 - Jan 2019*

Advisor: Sheng-Hsien Chiu

Research Experience

Tabor group, Chemistry Department, TAMU — *College Station, TX*

Graduate Research Assistant — *Oct 2019 - Current*

- Designed machine learning models (Graph Neural Network, Gaussian Process Regression) for molecular property prediction and high-throughput virtual screening for organic electronics.
- Maintained PostgreSQL database and software package for high-throughput virtual screening in the research group.
- Developed methods using molecular dynamics simulation and electronic structure calculation for elucidating structure–property relationships of redox-active polymers for organic battery design.
- Mentored two undergraduate students, teaching them molecular dynamics simulations and the basics of electronic structure.

Chiu group, Chemistry Department, NTU — *Taipei, Taiwan*

Undergraduate Research Assistant — *Jul 2016 - Feb 2019*

- Synthesized water-soluble [2]rotaxane using the clipping method.

Awards

2022 **Departmental Travel Award**, Chemistry Department, TAMU — *College Station, TX*

2022 **Air Force Scholarship**, American Conference on Theoretical Chemistry — *Tahoe, CA*

2018 **Undergraduate Research Project Grant**, Ministry of Science and Technology — *Taiwan*

Publications

1. **C.-H. Li**, D.P. Tabor, Accelerating Organic Electronic Materials Design with Low-Cost Molecular Reorganization Energy Predictions, *in preparation*
2. T. Ma, **C.-H. Li**, R.M. Thakur, D.P. Tabor, J.L. Lutkenhaus, Uncovering the Origin of the Electrolyte's Role in Metal-free, Aqueous Radical Batteries, *in revision*
3. **C.-H. Li**, D.P. Tabor, Discovery of lead low-potential radical candidates for organic radical polymer batteries with machine-learning-assisted virtual screening, *J. Mater. Chem. A* **10**, 8273-8282 (2022).

Presentations

Contributed Talk

1. Inverse Design of Organic Radical Batteries with Redox-Active Polymers for Energy Storage through Multi-scale Modelling, Texas A&M Conference on Energy. September 2022. College Station, TX.

Poster Presentations

2. Accelerating Design of Redox-Active Polymers for Organic Radical Batteries by Machine-Learning-Assisted Virtual Screening and Insights from Molecular Simulations, American Conference on Theoretical Chemistry. July 2022. Tahoe, CA.
3. Leveraging Molecular Simulation to Analyze and Design Redox-Active Polymers for Energy Storage, Molecular Systems Design & Engineering Symposium. June 2021. (Virtual Poster).

Skills

Programming Languages Python, Shell scripting, SQL

Software Knowledge PyTorch, PostgreSQL, Django, Git

Computational Chemistry LAMMPS, GROMACS, VMD, Q-Chem, Gaussian, NWChem, ORCA, MDAnalysis, RDKit