Zhihao Feng

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PROFESSIONAL SUMMARY

Polymer-focused computational researcher building physics-grounded ML and simulation workflows spanning DFT, TDDFT, atomistic MD, and coarse-grained MD, especially for polymer semiconductors and sustainable polymers. Developed a physics-informed PRISM surrogate from 370+ GB CGMD data (∼400 systems; SANS-validated; > 90% benchmark wins) and built *pyForceTune* to optimize force fields against DFT reference data (46% lower binding-energy error; < 0.1 kcal/mol dihedral error).

EDUCATION

Georgia Institute of Technology Atlanta, GA — 2021 – 2025
Ph.D. in Chemical Engineering (Minor: Data Science for the Chemical Industry)
Advisors: Prof. Seung Soon Jang and Prof. Natalie Stingelin

Cornell University Ithaca, NY — 2019 – 2021
M.S. in Chemical Engineering
Advisors: Prof. Rong Yang and Prof. Jeffrey D. Varner

University at Buffalo, SUNY Buffalo, NY — 2017 – 2019
B.S. in Chemical Engineering and B.A. in Chemistry (*Summa Cum Laude*)
Advisor: Prof. Haiqing Lin

RESEARCH EXPERIENCE

Ph.D.: Polymer data/representation pipelines, DFT/MD simulation, and ML

- **ML-ready CGMD descriptors and physics-informed PRISM surrogate for polymer property/function (CGMD; ML; PRISM):** Developed an automated CGMD data/descriptor pipeline (**370+ GB**, ∼**400** systems) and trained a physics-informed ML closure (*TensorFlow*) to predict polymer correlation functions and derived properties; outperformed standard analytical closures in > 90% of tests, validated vs. SANS, and deployed an interactive tool for rapid inference in minutes vs. MD in hours to days (***JCP*, in revision (preprint)**)
- **Force-field optimization toolkit for reliable conjugated polymer simulations (DFT; MM; MD):** Developed ***pyForceTune***, a Python (*Pyomo*) toolkit to optimize bonded and nonbonded parameters against DFT reference data (*Jaguar*); reduced binding-energy errors by **46%** vs. general force fields and achieved < 0.1 **kcal/mol** dihedral error vs. DFT (***JACS*, in prep; *SPIE Proc.*, 2025**)
- **Simulation-to-descriptor workflows tied to experiments (DFT; MD; Debye scattering):** Conducted vibrational simulations (for example, Raman and IR) in DFT, performed conformational sampling, and computed Debye scattering from MD trajectories across > 30 conjugated polymer/small-molecule systems; extracted conformation/packing signatures to connect simulations to thin-film experimental observables (***Nat. Energy*, *Nat. Mater.*, *Adv. Mater.* submitted; *Solar RRL*, *Mater. Horiz.***)
- **Large-scale polymer simulation for thermodynamics (MD; Debye scattering):** Ran large-scale all-atom MD in *LAMMPS* (> 15,000 **atoms**, > 400 **ns**) across temperature schedules, calculated order/alignment parameters, and computed absolute entropy (2PT); identified drivers of assembly and thermal transitions to guide processing/stability decisions (**in prep**)
- **Conformation-ensemble electronic disorder analysis (DFT; MD):** Combined MD conformational sampling with DFT electronic-structure calculations to quantify dynamic electronic disorder and identify structural motifs that control disorder trends (***Nat. Chem.* submitted**)
- **Benchmarking ML interatomic potentials for accelerated atomistic simulation (UMA; MACE):** Fine-tuned and evaluated UMA and MACE-class interatomic potentials (*MatterTune*) on domain-relevant structures; improved readiness for high-throughput atomistic simulation and rare-event settings.
- **Electronic-structure features linked to polymer conformations (TDDFT; NTO):** Conducted TDDFT/NTO analysis in DFT across > 7 conjugated polymers/small molecules and polyurethane systems; connected structural changes to excited-state character to support stability and optical-property interpretation (***ACS Appl. Mater. Interfaces* submitted; *Prog. Org. Coatings*, 2025**)
- **ML-driven screening under limited compute (MD/MC; SMILES/RDKit; Bayesian optimization):** Built a high-throughput MD/MC pipeline to curate a 1,000+ polyamine dataset and ML-ready representations

(SMILES/RDKit + BRICS/RECAP; polyBERT/PolyNC embeddings) and implemented Bayesian optimization for budget-aware candidate selection ($N_0 = 10$, **budget** $= 30$; **20** retrospective runs); prioritized high-performing candidates from a ∼1,000-compound pool (***EES*, in prep**)

- **Graph-based trajectory analysis for tortuosity (MD):** Constructed per-frame atomistic connectivity graphs from MD trajectories; sampled source/target atoms and computed shortest-path lengths to quantify transport tortuosity in polymer bulk and slab morphologies.
- **Mechanical response modeling (MD):** Modeled stress–strain behavior of conjugated polymers; quantified how chemical design and entanglement influence stretchability and toughness.
- **Interface modeling for sustainable materials (MD):** Simulated PDMS–water and PDMS–octane interfaces; quantified surface tension and interfacial ordering to inform multi-surface repellency design.

M.S.: ML-guided polymer discovery

- **Virtual screening for antibiofilm polymers (SMILES/RDKit; ML):** Built a virtual screening pipeline for **2,000**+ amphiphilic copolymers using SMILES and RDKit-derived features and trained an ensemble model combining SVR with autoencoder-derived latent representations; identified and experimentally validated high-performance antibiofilm polymers (***Adv. Mater. Technol.*, 2023**).

COMPUTATIONAL SKILLS

Languages:	Python, R, Bash, Git
Key libraries:	TensorFlow, RDKit, Pyomo, SciPy, MDAnalysis, Two-Phase Thermodynamics, MatterTune
Software:	Schrödinger (Maestro, Jaguar), Gaussian, VASP, Materials Studio, LAMMPS
Infrastructure:	HPC/Slurm, GPU computing

PUBLICATIONS AND MANUSCRIPTS

Peer-reviewed articles

[1] Jae Hoon Son, Keren Ai, Jaehyeong Kim, **Zhihao Feng**, Rose Newman, Yeonjeong Lee, Jongmin Han, Myong Hoon Song, Seung Soon Jang, Jin Young Kim, James R. Durrant, and Han Young Woo. "Redefining molecular design and exciton dynamics in single-component organic photocatalysts for efficient solar-to-hydrogen conversion." **Co-first author;** ***Materials Horizons, 2026***

[2] Minse Kim, Md Morshedur Rahman, Sung Hyun Kwon, **Zhihao Feng**, Nazrul Hsan, Ingi Hong, Seung Soon Jang, and Joonseok Koh. "Synthesis and properties of colored waterborne polyurethanes containing a uracil azo moiety: Experimental and computational study." ***Progress in Organic Coatings 2025, 211, 109751***

[3] Maria G. D. Guaita, Rodrigo Szostak, Francisco M. C. da Silva, **Zhihao Feng**, Lucas Scalon, Verônica C. Teixeira, Antônio A. M. Gasperini, Tim Kodalle, Carolin M. Sutter-Fella, Seung Soon Jang, Hélio C. N. Tolentino, and Ana F. Nogueira. "Revealing the Crystallization Pathways of Mixed-Halide Low-Dimensional Perovskites: A First Step Toward Solar Cell Applications." ***Solar RRL, 2025, 9:e2500404***

[4] **Zhihao Feng**, Yifan Cheng, Alexandra Khlyustova, Aasim Wani, Trevor Franklin, Jeffrey D. Varner, Andrew L. Hook, and Rong Yang. "Virtual High-Throughput Screening of Vapor-Deposited Amphiphilic Polymers for Inhibiting Biofilm Formation." ***Advanced Materials Technologies 2023, 8, 13, 2201533***

[5] Xiaoyi Chen, **Zhihao Feng**, Janavi Gohil, Christopher M. Stafford, Ning Dai, Liang Huang, and Haiqing Lin. "Reduced Holey Graphene Oxide Membranes for Desalination with Improved Water Permeance." ***ACS Applied Materials and Interfaces 2020, 12, 1, 1387–1394***

Manuscripts in review/revision

[6] **Zhihao Feng**, Christian T. Randolph, Tyler B. Martin, and Thomas E. Gartner III. "A Machine Learning Closure for Polymer Integral Equation Theory." **In revision at** ***Journal of Chemical Physics***

[7] Pang Wang, **Zhihao Feng**, Huiyue Ping, Florian Zimmermann, Seren Dilara "Oz, Chen Chen, Wei Li, Ahmed Kadid, Maximilian Schiffer, Yang Liu, Daan Coenen, Guorui He, Timo Maschwitz, Christian T"uckmantel, Felix Lang, Wouter Maes, Yinhua Zhou, Tao Wang, Selina Olthof, Seung Soon Jang, Kai O. Brinkmann, and Thomas Riedl. "Disentangling Degradation of Non-Fullerene Organic Solar Cells in Air." **Co-first author (corresponding author); In revision at *Joule***

[8] Min Gyu Kang, Rose Newman, **Zhihao Feng**, Charlie Jeffreys, Jae Hoon Son, Jinwoo Lee, Min Hun Jee, Lingyun

Zhao, Stanley Cazaley, Seung Soon Jang, James R. Durrant, and Han Young Woo. "Core Alkyl-Chain Engineering Programs Lattice-Ordered Nonfullerene Acceptor Nanoparticles for Efficient Single-Component Photocatalytic Hydrogen Evolution." **Co-first author; In revision at *ACS Nano***

[9] Henry J. Kantrow, Hongmo Li, Elizabeth Gutiérrez-Meza, **Zhihao Feng**, Spencer Yeager, Yael Tsarfati, Karen C. Bustillo, Peter Ercius, Xabier Rodríguez Martinez, Xingyuan Shi, Christina Cheng, Anna Kyrri, Luke Balhorn, Félix Thouin, Hao Li, Antonio Facchetti, Jenny Nelson, Jaime Martin, Qiao He, Martin Heeney, Sophia C. Hayes, Renaud Demadrille, Alberto Salleo, Sergei Tretiak, Erin L. Ratcliff, Seung Soon Jang, Carlos Silva-Acuña, and Natalie Stingelin." **In review at *Nature Chemistry***

[10] Hongmo Li, Henry J. Kantrow, David Valverde-Chávez, Olivier Bardagot, **Zhihao Feng**, Jaden Cramlet, Sebastian Toyotoshi, Cyril Aumaitre, Antoine Curé, Seung Soon Jang, Alberto Salleo, Erin Ratcliff, Stephen Barlow, Renaud Demadrille, Seth R. Marder, Carlos Silva, and Natalie Stingelin. "Using vitrification to predict molecular limits for conjugated polymer:dopant interactions." **In review at *Nature Materials***

[11] Hongmo Li, Henry J. Kantrow, David Valverde-Chávez, Meghan McNeil, Arianna Magni, Mohammad Balooch Qarai, Jude Kpare, Jaden Cramlet, Qiao He, Félix Thouin, **Zhihao Feng**, Andrew Comstock, Stephen Barlow, Jason Azoulay, Seung Soon Jang, Renaud Demadrille, Martin Heeney, Seth Marder, Nick Hestand, Alberto Salleo, Frank C. Spano, Carlos Silva-Acuña, and Natalie Stingelin. "Trions as fundamental species in chemically doped polymer semiconductors." **In revision at *Advanced Materials***

[12] Md Morshedur Rahman, Sehun Kim, Sunghyun Kwon, **Zhihao Feng**, Nazrul Hsan, Seunga Choi, Ingi Hong, Seung Soon Jang, and Joonseok Koh. "Intrinsically Neutral Black Waterborne Polyurethane Membranes via TD-DFT-Guided Covalent Chromophore Integration." **In review at *ACS Applied Materials & Interfaces***

[13] Indunil Angunawela, Subhrangsu Mukherjee, Somayeh Kashani, **Zhihao Feng**, Seung Soon Jang, and Harald Ade. "Mesophase ordering in ABA or ABA′ transverse amphiphilic semiconducting polymers." **In review at *Advanced Functional Materials***

Manuscripts in preparation

[14] **Zhihao Feng**, Henry J. Kantrow, Jinwon Cho, Junhe Chen, Omar Allam, Sunghyun Kwon, Jiil Choi, Harald Ade, Natalie Stingelin, and Seung Soon Jang. "*pyForceTune*: A General Force Field Optimization Package for Semiconducting Polymers." **In preparation for *Journal of the American Chemical Society***; related proceedings: ***SPIE Proc.*, 2025**

[15] **Zhihao Feng**, Henry J. Kantrow, Mark D. Weber, Natalie Stingelin, and Seung Soon Jang. "Molecular Origin of Mesophase Transitions in pBTTT Revealed by Multiscale Modeling." **In preparation**

[16] Junhe Chen, Alif Qayyum, Nafiz Abeer, **Zhihao Feng**, Hyun Myung Woo, Seung Soon Jang, and Byung Jun Yoon. "Enabling Machine Learning-Assisted Discovery of Polyamines for Solid-State CO_2 Capture." **Co-first author; In preparation for *Energy and Environmental Science***

[17] Pang Wang, Kai O. Brinkmann, **Zhihao Feng**, Seung Soon Jang, and Thomas Riedl. "Understanding the Stability Limits of PM6:Y6 Organic Solar Cells under UV Irradiation and Nitrogen Environment." **In preparation for *Nature Energy***

AWARDS AND HONORS

- 2026: PMSE Emerging Professional Award — 1 of 15 selected worldwide, ACS
- 2025: Computational Allocation Award, National Renewable Energy Laboratory
- 2025: Amyn S. Teja International Research Endowment Fund, Georgia Tech
- 2024: Best Poster Award, Center for Organic Photonics and Electronics, Georgia Tech
- 2024: Beamtime Allocation Award, Paul Scherrer Institute
- 2024: Travel Award, College of Engineering, Georgia Tech
- 2023: Poster Runner-Up, Student Polymer Network, Georgia Tech
- 2022: Ph.D. Student Exemplary Achievement Award, Georgia Tech
- 2019: Dean's Achievement Award, University at Buffalo
- 2019: Academic Excellence in Chemistry Award, University at Buffalo
- 2019: Travel Award, North American Membrane Society

- 2019: Scholarship, School of Engineering and Applied Sciences, University at Buffalo
- 2019: Dean's List, University at Buffalo
- 2018: Dean's List, University at Buffalo

PROFESSIONAL SERVICES

- 2024–2026: Student Leader, Designing Materials to Revolutionize and Engineer our Future (DMREF) Program, Georgia Tech, NC State, and NIST
- 2024–2026: Creator, DMREF Repository and Portfolio Website, Georgia Tech
- 2024–2025: Maintainer, Natalie Stingelin Group Website, Georgia Tech
- 2024–2025: Member, The Society for Photonics Instrumentation Engineers (SPIE) Student Chapter, Georgia Tech
- 2022–2023: Member, School of Chemical & Biomolecular Engineering Safety Council, Georgia Tech

CONFERENCE PRESENTATIONS

[1] Zhihao Feng, Natalie Stingelin, and Seung Soon Jang. Presentation (invited, scheduled), "Deciphering side-chain-functionalized polymer semiconductors: Insights on structure and thermal phase behavior from multiscale modeling." American Chemical Society Fall Meeting, Chicago, Illinois, USA, 2026.

[2] Zhihao Feng, Natalie Stingelin, and Seung Soon Jang. Presentation (contributed), "Thermal behavior of semiconducting polymer assembly using multiscale modeling approach." Society of Photo-Optical Instrumentation Engineers Optics + Photonics, San Diego, California, USA, 2025.

[3] Zhihao Feng, Henry J. Kantrow, Natalie Stingelin, and Seung Soon Jang. Poster, "Unraveling the Influence of Side-Chain Design on Semiconducting Polymer Assembly: Insights from Multiscale Modeling." International Conference on Organic Electronics, Coimbra, Portugal, 2025.

[4] Zhihao Feng, Henry J. Kantrow, Mark Weber, Jinwon Cho, Junhe Chen, Omar Allam, Jiil Choi, Tyler Martin, Sunghyun Kwon, Natalie Stingelin, and Seung Soon Jang. Presentation (contributed), "Unraveling the influence of side chain architectures on semiconducting polymer assembly: Insights from multiscale modeling." Fπ16 Symposium, Jeju, Korea, 2025.

[5] Zhihao Feng, Henry J. Kantrow, Jinwon Cho, Junhe Chen, Omar Allam, Sunghyun Kwon, Jiil Choi, Natalie Stingelin, and Seung Soon Jang. Presentation, "Unraveling the influence of side chain architectures on semiconducting polymer assembly: Insights from multiscale modeling." American Chemical Society Fall Meeting, Denver, Colorado, USA, 2024.

[6] Zhihao Feng, Jinwon Cho, Junhe Chen, Omar Allam, and Seung Soon Jang. Presentation, "Investigating the effect of sidechains on self-assembly of semiconducting polymer using a multiscale modeling approach." American Physical Society March Meeting, Minneapolis, Minnesota, USA, 2024.

[7] Zhihao Feng and Thomas E. Gartner III. Poster, "Development of a machine learning-based closure relation for polymer integral equation theory." American Physical Society March Meeting, Las Vegas, Nevada, USA, 2023.

[8] Zhihao Feng, Yifan Cheng, Alexandra Khlyustova, Aasim Wani, Trevor Franklin, Jeffrey D. Varner, Andrew L. Hook, and Rong Yang. Presentation, "Virtual high-throughput screening of vapor-deposited amphiphilic polymers for biofilm reduction with machine/deep learning." American Institute of Chemical Engineers Annual Meeting, Boston, MA, USA, 2021.