Changwen Xu

412-999-1188 | changwex@umich.edu | linkedin.com/in/changwenxu | github.com/ChangwenXu98

Education

University of Michigan — Ann Arbor, MI
Doctor of Philosophy in Mechanical Engineering — *May. 2027 (expected)*

Carnegie Mellon University — Pittsburgh, PA
Master of Science in Computational Materials Science and Engineering, GPA: 4.0/4.0 — *Dec. 2022*

South China University of Technology — Guangzhou, China
Bachelor of Engineering in Materials Science and Engineering, GPA: 3.96/4.0 — *Jun. 2021*

Publication

1. Wang, Y., **Xu, C.**, Li, Z., Barati Farimani, A., Denoise Pretraining on Nonequilibrium Molecules for Accurate and Transferable Neural Potentials, *J. Chem. Theory Comput.*, 2023, 19, 15, 5077–5087
2. **Xu, C.**, Wang, Y., Barati Farimani, A., TransPolymer: a Transformer-based language model for polymer property predictions, *npj Computational Materials*, 2023, 9, 64
3. Wang, L. (#), **Xu, C.** (#), Zhang, W., Zhang, Q., Zhao, M., Zeng, C., Jiang, Q., Gu, C., Ma, Y., Electrocleavage Synthesis of Solution-Processed, Imine-Linked, Crystalline Covalent Organic Framework Thin Films, *J. Am. Chem. Soc.*, 2022, 144, 20, 8961–8968. (# These authors contributed equally.)

Research Experience

Machine Learning Summer Internship — Remote
Redesign Science — *Jun. 2023 – Aug. 2023*

Improving ML Collective Variables with Energy-based Path Construction | *Python, MD*

- Constructed **Minimum Energy Path** for better **Machine-Learned Collective Variables** for sampling rare events by metadynamics
- Trained time-lagged autoencoder to learn CVs that capture the metastability in low dimensions
- Conducted **interpolations** in CV space between start and end state and minimized the energy along the path for better **transition path**
- Ran **MetaD** simulation using the ML-CVs and compared the results to those without energy-aware paths

Graduate Student Researcher — Pittsburgh, PA
Carnegie Mellon University — *Oct. 2021 – May. 2022, Aug. 2022 – Present*

Graduate Research Assistant — Pittsburgh, PA
Carnegie Mellon University — *May. 2022 – Aug. 2022*

Denoise Pre-training for Accurate and Transferable Neural Potentials | *Python, PyTorch, Neural Potential*

- Proposed **denoise** pretraining on **non-equilibrium** molecular conformations to achieve more accurate and transferable GNN potential predictions
- Finetuned the model pretrained on small molecules to improve performance on diverse molecular systems with remarkable **transferability**
- Demonstrated **data efficiency** of pretrained GNNs for large and complex molecular systems with limited training data

Transformer-based Language Model for Polymer Property Predictions | *Python, PyTorch, Language Model*

- Proposed **TransPolymer**, a **Transformer** based model for accurate and efficient polymer property predictions
- **Pretrained** with **Masked Language Modeling** on a large unlabeled dataset of polymer sequences for learning expressive representations
- **Finetuned** the pretrained model in different downstream prediction tasks, achieving the state-of-the-art (**SOTA**) results and surpassing baseline models by large margins in most cases
- Highlighted the model as a promising computational tool for understanding chemistry in a data science view

Undergraduate Student Researcher — Guangzhou, China
South China University of Technology — *Sep. 2018 – Jun. 2021*

Electrocleavage Synthesis of Solution-Processed Covalent Organic Framework (COF) Thin Films

- Developed an unprecedented electrocleavage synthesis strategy to produce **imine-linked COF films** directly on electrodes from electrolyte solutions at room temperature
- Carried out **cathodic exfoliation** of COF powders into nanosheets by electrochemical reduction and protonation and **anodic oxidation** to reproduce COF structures
- Characterized the COF films, COF solutions as well as precipitated COF nanosheets to verify the method

Synthesis and Solution Processing of Triazine-based Crosslinked Conjugated Polymers (TCPs)

- Reported the method of **protonating** the polymeric skeletons to enhance the solubility of TCPs under electrostatic repulsions to achieve solution processing
- Synthesized triazine-based n-type crosslinked conjugated polymers with **perylene diimide** units and achieved **solution-processing** of crosslinked conjugated polymers for the fabrication of polymeric films
- Developed the method of electrocleavage synthesis of triazine-based COFs from previous research and compared the results of the two methods.

Projects

AI Ramanujan: Discovery of Formula Equivalence (CMU) | *PyTorch, Language Model* Oct. 2022 – Present

- Train **Transformer** encoders to evaluate whether two mathematical formulas map to the same value
- Construct a **tokenizer trainer** for adaptation to formulas in Mathematica format and design a **translator** to convert formulas in Maple format into Mathematica format
- Adapt the encoders with **cross attention** to encode correlations between two embeddings and train the model by **contrastive learning**

JPX Tokyo Stock Exchange Prediction (CMU) | *Python, PyTorch, sklearn, EDA* May. 2022 – Jul. 2022

- Trained **LSTM** model for JPX stock prediction and compared the model against real future returns for evaluation
- Applied exploratory data analysis on JPX stock data, conducted data cleaning, and carried out **feature engineering** to construct financial descriptors
- Achieved the highest rank of top 15% in Kaggle competition "JPX Tokyo Stock Exchange Prediction"

Developing disaster relief and response system (SCUT) | *Python, MATLAB* Jan. 2019 – Jan. 2019

- Participated in 2019 Mathematical Contest in Modeling working on developing a feasible aerial disaster relief and emergency response system, and was designated as Meritorious Winner
- Determined the optimal drone fleet, payload packing configurations, and cargo container locations of the system
- Proposed **elliptic interpolation algorithm** to design delivery routes and schedules of flight plan

Invited Talks

Invited Speaker at "Math + Machine Learning + X" Seminar at Brown University Nov. 2022

- Gave a talk on *TransPolymer: a Transformer-based Language Model for Polymer Property Predictions*

Professional Service

Reviewer: NeurIPS'23, ML4Materials Workshop @ ICLR'23, SPIGM @ ICML'23

Honors and Awards

Outstanding Undergraduate of MSE, South China University of Technology	Jun. 2021
Xiaolan Wu Scholarship	Jun. 2021
Outstanding Undergraduate Thesis	Jun. 2021
Kemingda Scholarship	Oct. 2020
Hongping Changqing Foundation Scholarship	Jun. 2019 – Jun. 2020
National Scholarship (Twice) (0.2% among all the university students in China)	Dec. 2018 – Dec. 2019
First Prize (Guangdong) of China Undergraduate Mathematical Contest in Modeling	Nov. 2019
Meritorious Winner of Mathematical Contest in Modeling	Apr. 2019
Second Prize of "FLTRP" Cup English Writing Contest	Dec. 2018