

XINGYU (ALFRED) LIU

City View Apartments, 1420 Centre Avenue 1603, Pittsburgh, PA, 15219
412-482-2106 ♦ xingyu1@andrew.cmu.edu ♦ xingyuliu.me

EDUCATION

Carnegie Mellon University

Doctor of Philosophy in Materials Science & Engineering - GPA: 3.87/4.0

Pittsburgh, PA
December 2021 (expected)

Thesis: Looking for Singlet Fission Candidates with Machine Learning and Hierarchical Database Screening

Secondary Master of Science in Machine Learning

December 2021 (expected)

Carnegie Mellon University

Master of Science in Materials Science & Engineering - GPA: 3.81/4.0

Pittsburgh, PA
December 2017

Wuhan University of Technology

Bachelor of Science in Materials Science & Engineering - GPA: 91.11/100

Wuhan, Hubei, P.R.China
June 2016

GRADUATE RESEARCH

Many-Body Perturbation Theory Meets Machine Learning to Discover Singlet Fission Materials

Carnegie Mellon University

September 2018 – Present

- Designed the workflow for database screening after initial tests of samples. This project proposal was listed as an Early Science Project (ESP) at Argonne National Laboratory.
- Implemented band gap classifier and regressor using multiple structural descriptors paired with machine learning algorithms such as logistic regression and gaussian process regression.
- Acquired a regression model with lowest root mean square error as 0.45 eV, which is lower than the state-of-the-art model for molecular materials.
- Utilized the idea of active learning and implemented a framework of sampling process to change the imbalance condition of training data. Percentage of preferred class was increased from 3% to 6%.
- Trained high-fidelity thermodynamic driving force regressor using sure independence screening and sparsifying operator (*S/SSO*), achieving the lowest root mean square error as low as 0.17 eV.
- Identified multiple singlet fission candidate materials via screening public database. Published multiple papers.
- Collaborated with staff from Intel and Argonne National Laboratory to implement this workflow and prepared to port it into the next generation supercomputer Aurora.

ACADEMIC PROJECTS

Enhance the Band Gap Classifier for Organic Molecular Crystals with Batch Mode Active Learning

Carnegie Mellon University

April 2020 – June 2020

- Performed literature review to understand the status of batch-mode active learning (BMAL). Determined several schemes for BMAL for further study.
- Implemented the *Relevance, Diversity and Density* and *Fisher Information Matrix Reduction* schemes and decided *Fisher Information Matrix Reduction* is more informative given the same starting pool of structures.

Fully-Printable Perovskite Solar Cells

Wuhan University of Technology

October 2015 – June 2016

- Ran several tests and confirmed the best ration of $\text{CH}_3\text{NH}_3\text{Cl}$ into the perovskite precursor.
- Photoluminescence spectra shows the strongest intensity with 0.45 M $\text{CH}_3\text{NH}_3\text{Cl}$, indicating fewer traps and defects within the perovskite crystal, which is consistent with the power conversion efficiency peak.

TEACHING EXPERIENCE

Course Assistant - 24-623 Molecular Simulation of Materials, CMU

Fall 2017

- Hosted office hours and graded homework.

Course Assistant - 27-710 Quantum Mechanics of Materials, CMU

Spring 2019 & 2020

- Ran bi-weekly recitations, covered the omissions from the lectures.
- Collaborated with the lecturer and decided the progress of the course.

SKILLS

Python, PyTorch, Scikit-Learn, Matplotlib, C++, Data Analysis, Microsoft Office

WORK EXPERIENCE

Zhongfu Shenyang Carbon Fiber Co.,Ltd.

July 2015

Position: Quality Control Intern

- Collected carbon fiber examples from the production line and delivered it to testing center.
- Analyzed the testing results and drafted the testing report.
- Proposed practical methods to improve the product quality.

AWARDS & HONORS

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|---|-----------|
| • Department of Materials Science & Engineering MS Research Excellence Award, CMU | June 2017 |
| • First Prize in Hubei Province College Student Art Festival --- Instrumental Music, Hubei Province | June 2015 |

EXTRA-CURRICULAR

Carnegie Mellon Graduate Consulting Club

2018-2019

Position: VP of Case Competition

- Attended executive board meeting and discussed services offered to the club members.
- Organized the Pittsburgh Innovation Case Competition (PICC) in 2019.
- Received sponsorship from multiple firms including BCG.
- Collaborated with consultants from multiple firms including McKinsey and Deloitte and asked for their support serving as the judges of PICC.

Wuhan University of Technology Symphony Orchestra

2013-2015

Position: Head of Second Violin Group

- Established the first university symphony orchestra with my colleagues.
- Organized the weekly training of second violin group and monitor the performance of my group.
- Coordinated the commercial performances and competed in art festival.

PRESENTATIONS

- Liu, Xingyu. "Acene and Acene-like Derivatives as Intermolecular Singlet Fission Candidates." *GW goes large scale (GW-XL) Workshop*, Helsinki, Finland, 10 June 2020. Conference Presentation.
- Liu, Xingyu. "On the Possibility of Singlet Fission in Crystalline Quaterylene." *Hands-on DFT and Beyond: High Throughput Screening and Big-Data Analytics, Towards Exascale Computational Materials Science*, Barcelona, Spain, 27 August 2019. Poster Presentation.
- Liu, Xingyu. "Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission." *Simulators Annual Meeting*, Pittsburgh, PA, 15 May 2019. Conference Presentation.
- Liu, Xingyu. "Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission." *American Physics Society (APS) March Meeting*, Los Angeles, CA, 7 March 2018. Conference Presentation.

PUBLICATIONS

- Longbing Qu, Yunlong Zhao, Aamir Minhas Khan, Chunhua Han, Kalele Mulonda Hercule, Mengyu Yan, **Xingyu Liu** et al. Interwoven Three-Dimensional Architecture of Cobalt Oxide Nanobrush-Graphene@Ni_xCo_{2x}OH_{6x} for High Performance Supercapacitors. *Nano Lett.* 15, 3, 2037–2044, 2015.
- Huirong Jiang, **Xingyu Liu** et al. Alleviate the J–V hysteresis of carbon-based perovskite solar cells via introducing additional methylammonium chloride into MAPbI₃ precursor. *RSC Adv.* 8, 35157-35161, 2018.
- Xiaopeng Wang, **Xingyu Liu** et al. On the possibility of singlet fission in crystalline quaterylene. *J. Chem. Phys.* 148, 184101, 2018.
- Xiaopeng Wang, **Xingyu Liu** et al. Phenylated acene derivatives as candidates for intermolecular singlet fission. *J. Phys. Chem. C* 123, 10, 5890–5899, 2019.
- Xiaopeng Wang, Rithwik Tom, **Xingyu Liu** et al. An energetics perspective on why there are so few triplet–triplet annihilation emitters. *J. Mater. Chem. C* 1, 10.1039/d0tc00044b, 2020.
- Xingyu Liu** et al. Pyrene-stabilized acenes as intermolecular singlet fission candidates: Importance of exciton wave function convergence. *J. Phys. Condens. Matter.* 32(18), 2020.