

# Yi Yang

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## EDUCATION

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<b>Carnegie Mellon University</b> <i>Doctor of Philosophy in Materials Science and Engineering</i>	Pittsburgh, PA <i>Jan. 2023 – Present</i>
<b>Carnegie Mellon University</b> <i>Master of Science in Computational Materials Science and Engineering</i>	Pittsburgh, PA <i>Aug. 2021 – Dec. 2022</i>
<b>China University of Geosciences, Wuhan</b> <i>Bachelor of Science in Materials Science and Engineering (experimental class)</i>	Wuhan, China <i>Sept. 2017 – July 2021</i>

## PUBLICATIONS

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- [1] R. Tom, S. Gao, **Y. Yang**, K. Zhao, I. Bier, E. Buchanan, A. Zaykov, Z. Havlas, J. Michl, and N. Marom. “Inverse Design of Tetracene Polymorphs with Enhanced Singlet Fission Performance by Property-Based Genetic Algorithm Optimization.” *Chemistry of Materials*, 2023
- [2] **Y. Yang**, R. Tom, J. Moussa, and N. Marom. “Genarris 3.0: A Random Structure Generator for Molecular Crystals” [Under preparation]
- [3] K. Nayal-Singh, D. O’Connor, R. Zubatyuk, D. Anstine, **Y. Yang**, I. Bier, R. Tom, W. Deng, K. Tang, O. Isayev, and N. Marom. “Training the AIMNet Potential for Crystal Structure Prediction in the Seventh CSP Blind Test.” [Under preparation]

## HONORS & AWARDS

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<b>Award for Research Excellence in the Master Program</b>	May 2023
<b>ATK-Nick G. Vlahakis Graduate Fellowship</b>	Feb. 2023
<b>Outstanding Undergraduate of MSE, China University of Geosciences, Wuhan</b>	June 2021

## EXPERIENCE

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<b>Research Assistant</b> <i>Carnegie Mellon University, Advisor: Noa Marom</i>	Pittsburgh, PA <i>Sept. 2021 – Present</i>
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### **Co-Crystal Structure Prediction Using Genarris and GAtor with Machine Learned Potentials**

- Implemented machine-learned potentials to enhance efficiency in structure search and optimization during the generation
- Integrating the AIMNet training procedure with a random molecular structure generator (Genarris)

### **Development of Genarris3.0: A Random Molecular Structure Generator**

- Implemented memory efficient duplicate removal algorithm using MPI4Py
- Developed a structure optimization algorithm for molecular crystals to minimize crystal volume
- Assessed the cost vs accuracy of semi-empirical and machine-learned potentials for screening crystals
- Preparing a manuscript for Genarris3.0 paper

### **Inverse Design by Property-Based Genetic Algorithm Optimization**

- Relaxed and ranked the best structures generated by GAtor using PBE+MBD method within FHI-aims
- Analyzed interaction energy in molecular chains to compare Density Functional Theory (DFT) method performance
- Examined and illustrated the evolution of Genetic Algorithms using diverse fitness functions

### **The 7<sup>th</sup> Crystal Structure Prediction Blind Test**

- Performed Single Point Energy (SPE) evaluations on structures generated by Genarris using FHI-aims
- Ranked relative energies for various targets in Phase 2 of the blind test, comparing results from different DFT and AIMNet methods
- Preparing a manuscript for submission to the Special Blind Test Issue, targeting publication in *Acta Crystallographica*.

## PROJECTS

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### **AI Ramanujan - Discovery of Formula Equivalence (11-785 Course Project)(CMU)** Oct. 2022 – Dec. 2022

- Trained Transformer encoders to identify equivalent mathematical formulas
- Designed a translator to efficiently convert mathematical formulas from Maple to Mathematica format
- Enhanced the encoders with cross-attention mechanisms to capture correlations between embeddings
- Employed contrastive learning for model training to improve performance

### **JPX Tokyo Stock Exchange Prediction (CMU)**

May 2022 – July 2022

- Selected and led a Kaggle competition focused on analyzing the Tokyo market
- Developed a Long short-term memory (LSTM) model with PyTorch for predicting JPX stock trends
- Conducted exploratory data analysis on Tokyo stock market data to extract key financial features
- Achieved a top 13% ranking (283/2033) in this Kaggle competition

## TECHNICAL SKILLS

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**Languages:** English (Fluent), Chinese (Native Speaker)

**Libraries:** ASE, Pymatgen, PyTorch, TensorFlow, PySpark

**Parallel Programming and Cloud Computing:** MPI, AWS

**Computational Material Science:** FHI-aims, DFTB+

**High Performance Computing:** Bridges2 (PSC), Perlmutter (NERSC), Theta (ALCF)

**Misc Skills:** supervised and unsupervised ML models, deep learning models, Unix systems