

# Yi Cao

AI4Science | Computer-Aided Material Design | DFT | Molecular Dynamics | Machine Learning | 2D Materials

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## Education

- PhD**    **Johns Hopkins University**, Chemical and Biomolecular Engineering (ChemBE)    Sept. 2023 to Present
- GPA: 4.0/4.0
  - **Advisor:** Paulette Clancy
  - **Coursework:** Machine Learning, Artificial Intelligence, Modern Data Analysis, Intro Algorithms, Computing for Applied Maths, Modeling and Design of Chemical Processes, Interfacial Nano Systems, Thermodynamics & Stat Mech, Transport Phenomena
- BS**    **Fudan University**, Pharmacy    Sept. 2019 to July 2023
- GPA: 3.7/4.0 (Rank: 2/112)
  - **Awards:** “Graduate Star” Nomination Award (2023), Excellent graduates of Shanghai Colleges and Universities (2023), 1st Class Scholarship (2021), Shanghai Scholarship (2020)
- University of California, Berkeley**, Visiting Scholar    Aug. 2021 to Dec. 2021

## Research Experiences

- Johns Hopkins University**, Research under Advisor Paulette Clancy    MD, USA  
Nov. 2023 to present
- Focus on Bridging DFT and Machine-Learning for 2D Thermoelectrics Simulation and Rational Design.
  - **Skill set:** Machine learning, First-principles calculation, Molecular Dynamics (MD) simulation
- School of Engineering, Westlake University**, Summer Research    Hangzhou, China  
July 2022 to Aug. 2022  
2 months
- *The Role Protein Corona (PC) Plays in Brain-Targeted mRNA Delivery and the Further Manipulation for PC Optimization*
  - **Skill set:** nanoparticle characterization, protein engineering, animal experiments
- Institute of Science and Technology for Brain-inspired Intelligence, Fudan University**, Undergraduate Research    Shanghai, China  
Feb. 2022 to Jun. 2023  
16 months
- *Exploration of The Role That Hippocampal Dentate Gyrus (DG) Plays in the Transformation of Pain Components and its Mechanism*
  - **Skill set:** Neuro-pharmacology, Electrophysiology, Signal processing
- Pharmacology Research Group, School of Pharmacy, Fudan University**, Undergraduate Research    Shanghai, China  
Sept. 2020 to Jun. 2021  
10 months
- *Network Pharmacology Study on the Combination of Radix Salviae and Hedysarum Multijugum Maxim for Revealing the Mechanism of Hypertension*
  - **Skill set:** Meta-analysis, Protein-protein interaction (PPI), Cytoscape.

## Publications

- Low-energy pathways lead to self-healing defects in CsPbBr<sub>3</sub>**    2024  
<https://doi.org/10.1039/D5CP01641J> 

Kumar Miskin, **Yi Cao**, Madaline Marland, Farhan Shaikh, David T. Moore, John Marohn, Paulette Clancy\*

**Brain-targeted nanoparticle drug delivery systems: research advances.** Basic and Clinical Medicine, 42(1): 2-14. [10.3969/j.issn.1001-6325.2022.01.004](https://doi.org/10.3969/j.issn.1001-6325.2022.01.004) 

2022

**Yi Cao**, Chen Jiang\*

## Projects

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### **Unveiling Defect Tolerance and Self-Healing Mechanisms in Perovskite Solar Materials**

2023

- Investigated the intrinsic self-healing phenomena in metal halide perovskites, uncovering defect migration and recombination pathways.
- Combined DFT and transition state analysis to elucidate energy barriers associated with dominant defect dynamics.
- Identified defect configurations enabling long-term phase and photovoltaic stability, contributing to scalable perovskite solar cell design.

### **From Wastes to Watts: Machine-Learned Thermoelectrics via van der Waals Gap Engineering**

2024 – Present

- Constructing ML-enhanced interatomic potentials (MLFF) to model Cr-doped  $\text{Sb}_2\text{Te}_3/\text{CrTe}_2$  heterostructures, integrating quantum accuracy with MD scalability.
- Explored dopant-mediated van der Waals gap modulation to stabilize interlayer coupling and enable high-temperature operability.
- Predicted directional thermal transport using first-principles-calibrated Boltzmann transport models, offering insights into energy-harvesting device architectures.

## Conference Presentations

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### **Prognostics and Health Management (PHM) Society Annual Conference 2025**, Doctoral Symposium (Invited Participant)

Bellevue, WA, USA  
Oct. 26–31, 2025

- *Selected as 1 of 10 PhD students globally to present at the Doctoral Symposium*
- *Research focuses on data-driven diagnostics and physics-informed modeling for material failure prediction*

### **Artificial Intelligence for Materials Science (AIMS) Workshop, NIST**, Poster

Rockville, MD, USA  
Jul. 9-10, 2025

### **Quantum Matters in Materials Science Workshop, NIST**, Poster

Rockville, MD, USA  
Feb. 19-20, 2025

- *Topological Materials Engineering for Next-Generation Thermoelectrics*

### **ROSEI Summit 2025**, Poster

Baltimore, MD, USA  
Jan. 15, 2025

- *Tracing Cr Migration in  $\text{Sb}_2\text{Te}_3$  with Computational Simulation: Next-Generation Thermoelectrics Turning Waste Heat into Electricity*

### **Materials Research Society (MRS) Fall Meeting 2024**, Poster

Boston, MA, USA  
Dec. 1-6, 2024

- *Exploring Low-Energy Pathways for Self-Healing Defects in  $\text{CsPbBr}_3$ —A Computational Study*

### **Women in AI 2025**, Poster Presentation - Award Winner

Baltimore, MD, USA  
April. 9, 2025

- *Exploring Low-Energy Pathways for Self-Healing Defects in  $\text{CsPbBr}_3$ —A Computational Study*

## Additional Experience And Awards

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### **The JHU Teaching Institute 2025**

Baltimore, Maryland, USA  
June 2025  
Certificate

- Completed a program focused on enhancing teaching skills and pedagogical practices, presented by The Teaching Academy.

**Viva Biotech**

- Conducted Computer-Aided Drug Design (CADD) research using co-solvent MD simulations, optimizing drug discovery through protein-ligand interaction analysis.
- Collaborated with cross-functional teams to integrate computational insights into experimental workflows, enhancing the efficiency of the drug discovery pipeline.

Shanghai, China  
Jun. 2024 to Jul. 2024  
Internship

**Fudan iGEM team, iGEM Competition**

- Guided experimental design, scientific documentation.
- Led brainstorming sessions and advised on scientific writing.
- Our team won a Gold Medal and Best Environmental Project title.

Shanghai, China  
Dec. 2022 to Nov. 2023  
Part-time, Advisor

**Boehringer Ingelheim**

- Led a team in developing a white paper on quality culture through research and interviews, resulting in improved company-wide quality guidelines.

Pudong, Shanghai, China  
Dec. 2022 to Feb. 2023  
Internship