

# HUA, PENG

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Research Interest: Multiphysics simulation, image segmentation using deep learning and AI

## EDUCATION

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**The Hong Kong University of Science and Technology, HKSAR**

**Sep 2021 - Present**

**Expected Graduation Date:**

**Aug 2026**

Ph.D. candidate in Nanoscience & Technology

RedBird PhD (top 5%)

**The Hong Kong University of Science and Technology, HKSAR**

**Sep 2020 - Aug 2021**

Master of Chemical & Biomolecular Engineering

School of Engineering Excellent Student (top 3%)

**GPA:** 3.86/4.3 (Excellent)

**University of Missouri-Columbia, U.S.A.**

**Aug 2016 – May 2020**

Bachelor of Chemical Engineering

Member of Tau Beta Pi (top 3%)

**GPA:** 3.89/4.0 (Magna Cum Laude)

## AWARDS AND HONORS

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Best TA Award, HKUST

2023-2024

RedBird PhD Award, HKUST

2021-2022

Excellent Student Scholarship in Chemical and Biomolecular Engineering, HKUST

2020-2021

Magna Cum Laude Honors, University of Missouri-Columbia

2020

Honors Scholar, University of Missouri-Columbia

2020

Chemical Engineering Development Scholarship, University of Missouri-Columbia

2019-2020

Chan Scholarship in Chemical Engineering, University of Missouri-Columbia

2019-2020

High Dean's Honor Roll, University of Missouri-Columbia

2017-2020

Undergraduate Honor Research, University of Missouri-Columbia

2019

## RESEARCH EXPERIENCES

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**Modeling of Field-Driven Granular Collective Dynamics**

**Sep 2023 - Present**

*Supervisor: Prof. Yilong Han*

*HKUST*

- Developed a hybrid machine vision framework (YOLO-Unet-OpenCV) for high-speed granular tracking, achieving >95% segmentation accuracy under magnetic interference.
- Simulated collective bead motions via COMSOL & C++ simulation, coupling electromagnetic fields, contact mechanics, and fluid-structure interactions to resolve self-organized pattern formation.

**Multiscale Dynamics of Magnetically Programmable Confined Systems**

**Sep 2021 - Present**

*Supervisor: Prof. Yilong Han*

*HKUST*

- Simulated 2D phase transitions in binary system via LAMMPS, revealing critical melting dynamics and defect evolution under thermal gradients.
- Engineered 50-nm accuracy E-beam lithography nanoparticles for enhanced thermal dissipation, achieving 40% heat transfer efficiency matching COMSOL electro-thermal predictions.

- Assembled SU8-based microrobots via photolithography, enabling magnetic-field-driven collective shape morphing for targeted drug delivery with 1  $\mu\text{m}$  spatial precision.
- Designed a monolayer-confined microchannel (depth = 1  $\mu\text{m}$ ) to spatially confine micron-scale particles in 2D, enabled precise probing of low-dimensional dynamics.

### Machine Learning in Calcium Carbonate Nucleation Mechanism

Sep 2020 - Jul 2021

Supervisor: Prof. Richard Lakerveld

HKUST

- Developed a conductivity-based kinetic assay for  $\text{CaCO}_3$  nucleation in supersaturated solutions, correlating ion depletion rates with amorphous-to-crystalline phase transitions
- Trained an ensemble learning algorithm (MATLAB) on multimodal data (conductivity/pH/temperature), predicting dominant nucleation pathways (dense liquid phase vs. direct ion attachment) with >92% accuracy.

### Machine Learning Assisted Discovery in Porous Carbon

Sep 2018 - Jul 2020

Supervisor: Prof. Jian Lin

University of Missouri-Columbia, U.S.A.

- Constructed a database of 2,100+ porous carbon samples with 12 descriptors (SSA: 200–3,500  $\text{m}^2/\text{g}$ , PSD: 0.5–50 nm, surface functionalities) for methane uptake prediction ( $\pm 3.5\%$  error vs. experimental).
- Developed a hybrid MLP-GBDT model trained on  $\text{CO}_2$  adsorption isotherms to predict  $\text{CO}_2/\text{CH}_4$  selectivity ratios, achieving 90% accuracy in identifying top-performing materials for natural gas purification.

### Electrochemical Performance of Cathode Material

Aug 2018 - Aug 2019

Supervisor: Prof. Yangchuan Xing

University of Missouri-Columbia, U.S.A.

- Conducted experiments including preparing and synthesizing  $\text{LiMn}_{0.4}\text{Ni}_{0.4}\text{Co}_{0.2}\text{O}_2$  layered compounds, assembled coin cells under vacuum condition, operated *ARBIN* battery tester independently.
- Selected material characterization methods and analyzed test data (MATLAB) independently.

## PUBLICATIONS

- **Peng Hua**, Yilong Han, “Searching for various melting scenarios of 2D crystals”, *Matter* 7.1 (2024): 19-22. (Impact factor: 18.9)
- Chi Zhang, Dawei Li, **Peng Hua**, Jian Lin, “Machine learning assisted rediscovery of methane storage and separation in porous carbon from material literature”, *Fuel* 290 (2021): 120080. (Impact factor: 7.5)
- **Peng Hua**, Yilong Han, “Magnetic-field-induced crystal-hexatic-liquid-crystal transition in 2D binary crystals”, (under revision)
- **Peng Hua**, Yilong Han, “Antihyperuniformity Emergence at the Hexatic Criticality in 2D Melting”, (under preparation)

## SKILLS

<b>Language Skills</b>	Mandarin, Cantonese, English, German
<b>Computer Languages</b>	C, C#, C++, Python, JAVA, Swift, MatLab
<b>Software Skills</b>	Aspen Plus, Sprint, SolidWorks, AutoCAD, COMSOL, Sketchup, Blender, LAMMPS, Adobe After Effects, Adobe Audition, Premiere
<b>Processing Skills</b>	Photolithography, E-beam lithography, Nanoscribe 3D printing, optical tweezers, image recognition & segmentation, molecular dynamics (MD) simulation, multi-physics (optical, magnetic/electric field, fluid dynamics) simulation, 2D & 3D product rendering, animation rendering