Xiangyu Yin

 Lemont IL | ✉ xyin@anl.gov | 🌐 xiangyu-yin.com

EXPERIENCE

Argonne National Laboratory   Oct. 2023 – present
Postdoctoral Appointee   Lemont, IL

- Working on computational imaging technologies such as XRF, XRD, ptychography and tomography
- Conducting research on automatic experimentation and data analysis, utilizing cutting edge AI technologies
- Collaborating with beamline scientists to facilitate data processing and analysis for APS users

Toyota Research Institute   May 2022 – Aug. 2022
Research Intern   Los Altos, CA

- Developed a new reinforcement learning (RL) based catalysts design method, results in a utility patent submission, now internally utilized by the Energy & Environment team

University of British Columbia   Jul. 2017 – Sept. 2017
MITACS Globalink Research Intern   Vancouver, BC

EDUCATION

Carnegie Mellon University   2018 – 2023
Ph.D. in Chemical Engineering   Pittsburgh, PA

Tianjin University   2014 – 2018
B.S. in Chemical Engineering   Tianjin, China

RESEARCH

Autonomous Scientific Discovery   Oct. 2023 – present

- Enabled automatic X-ray Fluorescence (XRF) data analysis via automatic differentiation framework `MapsTorch`
- Improved ptychography efficiency and reconstruction quality via physics-informed Bayesian optimization
- Developed a foundation AI powered automation framework `nodeology` for building intelligent scientific workflows

Carbon Capture System Modeling   Jan. 2022 – Sept. 2023

- Identified the funding opportunity and co-wrote the project proposal to win the award from the DOE
- Proposed a novel surrogate learning workflow for solid adsorbents (i.e., MOFs) adsorption isotherms
- Developed a packed-bed adsorption column model for pressure swing adsorption (PSA) processes

Supply Chain Optimization   Dec. 2021 – Jan. 2022

- Developed a derivative-free optimization (DFO) algorithm for delivery schedule optimization

Crystalline Nanomaterials Design   Mar. 2019 – Dec. 2021

- Proposed a novel mathematical optimization-based crystalline nanomaterials design paradigm
- Carried out optimization-based design studies for nanoclusters, catalytic surfaces, nanowires and perovskites
- Developed `MatOpt` package to streamline the optimization-based nanomaterials design process

PUBLICATIONS

X. Yin, Z. Di, O. Antipova, S. Chen, Y. Jiang, and A. Glowacki. MapsTorch: Automatic Differentiation for X-ray Fluorescence Data Analysis. *In preparation*, 2024

X. Yin, C. Shi, Y. Han, and Y. Jiang. PEAR: A Robust and Flexible Automation Framework for Ptychography Enabled by Multiple Large Language Model Agents. ArXiv, 2024

X. Yin, L. Biegler and C. E. Gounaris. Inverse Design of Metal-Organic Frameworks for Adsorption Processes: Learning Algebraic Surrogate Models of Isotherm Parameters. *Submitted*, 2024

X. Yin and C. E. Gounaris. Computational Discovery of Metal-organic Frameworks for Sustainable Energy Systems: Open Challenges. *Computers & Chemical Engineering*, 2022

C. L. Hanselman, **X. Yin**, D. C. Miller, and C. E. Gounaris. Matopt: A python package for nanomaterials design using discrete optimization. *Journal of Chemical Information and Modeling*, 2022

X. Yin and C. E. Gounaris. Search methods for inorganic materials crystal structure prediction. *Current Opinion in Chemical Engineering*, 2022

X. Yin, N. M. Isenberg, C. L. Hanselman, J. R. Dean, G. Mpourmpakis, and C. E. Gounaris. Designing stable bimetallic nanoclusters via an iterative two-step optimization approach. *Molecular Systems Design & Engineering*, 2021

Z. Zhang, **X. Yin**, C. Zhu, Y. Ma, and T. Fu. Self-assembly of bubble swarm in large cavities in step-type parallelized microchannels and its feedback on bubble formation. *Chinese Journal of Theoretical and Applied Mechanics*, 2020

TALKS

X. Yin, Z. W. Di, O. Antipova, S. Chen, Y. Jiang and A. Glowacki. Automating X-ray Fluorescence Mapping with Differentiable Modeling. *Microscopy & Microanalysis*, 2024

X. Yin, C. Shi, J. Deng, Y. Han and Y. Jiang. PEAR: A Knowledge-guided Autonomous Pipeline for Ptychography Enabled by Large Language Models. *Microscopy & Microanalysis*, 2024

X. Yin, Z. Yang, Y. Han and Y. Jiang. Pushing the Limits of Electron Ptychography with Physics-informed Bayesian Optimization. *Microscopy & Microanalysis*, 2024

Y. Jiang, **X. Yin**, C. Zhen and Y. Han. Optimizing Parameters for High-resolution and Low-dose Ptychography. *APS March Meeting*, 2024

X. Yin, L. T. Biegler, and C. E. Gounaris. Incorporating Materials Surrogate Models into Process Models for Adsorption-Based Gas Separations. *AIChE Annual Meeting*, 2022

X. Yin, L. T. Biegler, and C. E. Gounaris. Enabling Process-materials Co-optimization via Surrogate Modeling for Adsorption-Based Gas Separations. *INFORMS Annual Meeting*, 2022

X. Yin, L. T. Biegler, and C. E. Gounaris. Towards process-materials co-optimization: Automatic generation of optimizable MOF structure-function relationships. *AIChE Annual Meeting*, 2021

X. Yin, C. L. Hanselman, D. C. Miller, and C. E. Gounaris. Matopt: A mathematical optimization-based nanomaterials design toolkit. *INFORMS Annual Meeting*, 2020

X. Yin, C. L. Hanselman, and C. E. Gounaris. Designing stable semiconductor nanowires via a generic materials optimization toolkit. *AIChE Annual Meeting*, 2020

X. Yin, C. L. Hanselman, D. C. Miller, and C. E. Gounaris. Nanomaterials design using Pyomo. *INFORMS Annual Meeting*, 2020

X. Yin, N. M. Isenberg, M. G. Taylor, G. Mpourmpakis, and C. E. Gounaris. Identification of stable bimetallic nanoclusters via a mathematical optimization framework. *AIChE Annual Meeting*, 2019