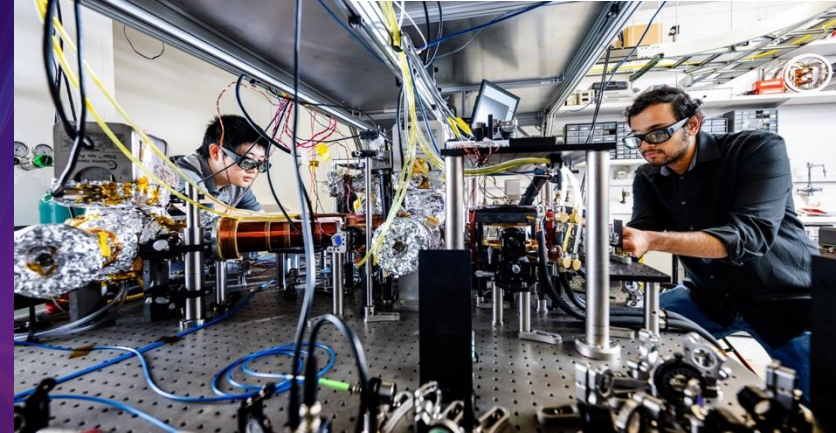


GENERATIVE AI, AGENTS, EXASCALE COMPUTING, AND LEADERSHIP CLASS USER FACILITIES FOR THE ACCELERATED DISCOVERY AND SYNTHESIS OF ENERGY MATERIALS



ELIU HUERTA

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HPC4Manufacturing
Livermore, California
February 24-26, 2026

CHALLENGE

Better mechanisms
for energy
storage and
conversion

Accelerated AI-
driven discovery of
novel energy
materials

**Because experimental
chemistry is time
consuming and costly,**
only handful of
materials have been
discovered and
commercialized for
energy storage and
conversion at
industrial scale

**Energy
independence**
requires using
domestic resources

**Design options
are vast;** need
to streamline

SOLUTION

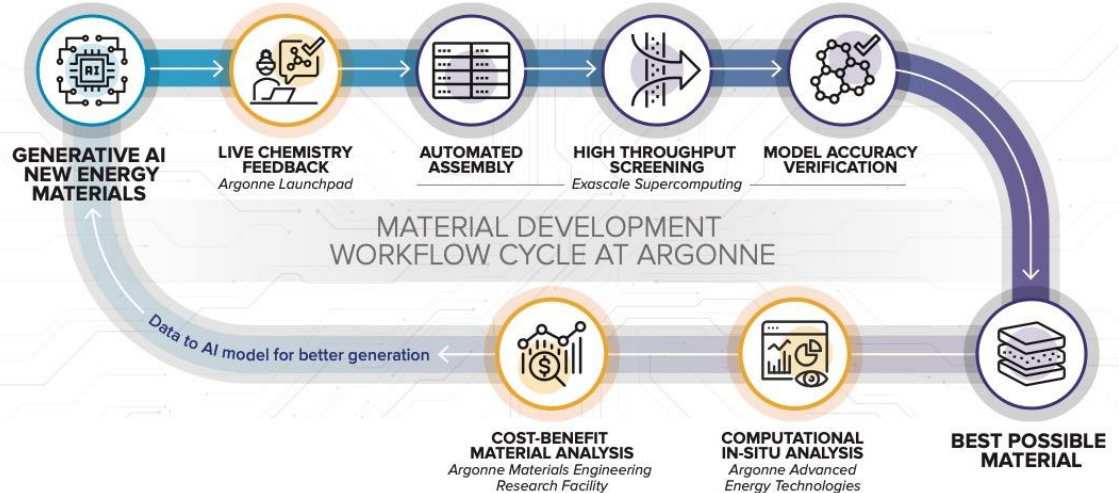
Combine computational chemistry, AI, and exascale computers with experimental chemistry

Focus on characterization, synthesis and cost analysis to deliver novel materials

Develop novel workflow at scale for industry

USING ARTIFICIAL INTELLIGENCE TO ACCELERATE MATERIAL RESEARCH

Argonne 
NATIONAL LABORATORY



 U.S. DEPARTMENT OF ENERGY Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC

ARGONNE CAPABILITIES

ALL UNDER ONE ROOF



HPC

High Performance
Computing

Polaris, Aurora, Equinox,
Solstice, Minerva, Janus,
and Tara



ALCF

Argonne Leadership
Computing Facility

In silico discovery at scale



MERF

Materials Engineering
Research Facility

Materials synthesization



APS

Advanced
Photon Source

Materials Characterization

WORLD-CLASS COMMUNITY OF TALENT IN MATERIALS SCIENCE

CASE STUDY | HPC4EI PROJECT WITH TOTAL ENERGIES

A generative artificial intelligence framework based on a molecular diffusion model for the design of metal-organic frameworks for energy conversion*

AI-Driven MOF Design

Researchers developed MOFA, an AI platform that generates and evaluates metal-organic frameworks (MOFs) for energy conversion combining AI-designed organic linkers with metal nodes

Rigorous Screening and Testing

The platform ensures MOFs are unique, synthesizable, and structurally valid, followed by simulations to assess their stability, chemical consistency, and adsorption capacities

Breakthrough Results

MOFA identified six novel MOFs with superior adsorption capacities, outperforming 96.9% of existing MOF datasets, showcasing the potential of AI for advancing energy storage technologies

*Hyun Park, Xiaoli Yan, Ruijie Zhu, **E. A. Huerta**, Santanu Chaudhuri, Donny Cooper, Ian Foster, Emad Tajkhorshid. *Nature Communications Chemistry* 7, 21 (2024)

HPC4EI PROJECT WITH TOTALENERGIES

Article | [Open access](#) | Published: 14 February 2024

A generative artificial intelligence framework based on a molecular diffusion model for the design of metal-organic frameworks for carbon capture

[Hyun Park](#), [Xiaoli Yan](#), [Ruijie Zhu](#), [Eliu A. Huerta](#) , [Santanu Chaudhuri](#), [Donny Cooper](#), [Ian Foster](#) & [Emad Tajkhorshid](#)

[Communications Chemistry](#) 7, Article number: 21 (2024) | [Cite this article](#)

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Associated content

Collection

Top 25 downloaded papers of 2024

Collection

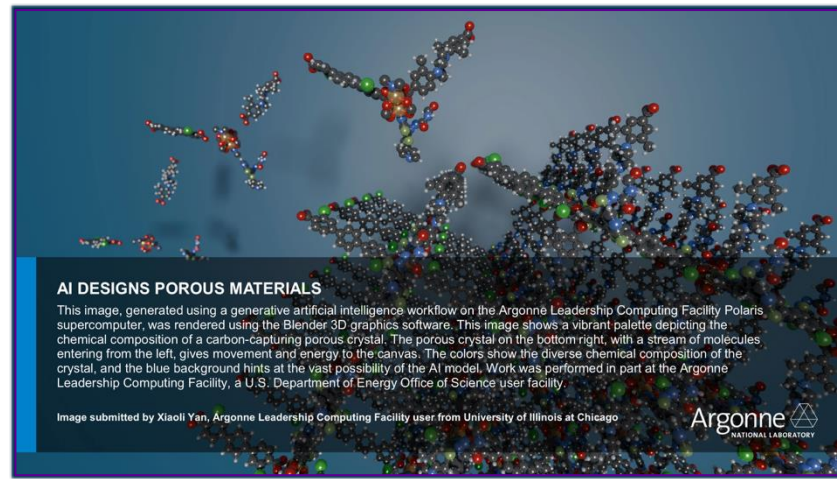
2024 Editors' Highlights

Featured as the cover of Nature Communications Chemistry and included in a mural exhibit in the Department of Energy building in Washington, D.C., outside the Secretary's office in 2024



Editors' Choice Awards

Argonne National Laboratory, the University of Chicago, and the Beckman Institute at the University of Illinois at Urbana-Champaign, and University of Illinois Chicago scientists combined generative AI, high throughput screening methods, and large-scale molecular dynamics simulations (with the LAMMPS code) to assemble, within seconds, novel, stable, and high-capacity metal-organic frameworks for carbon capture.



Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

FOR YOU

Refined computational workflow

- AI-driven discovery workflow works optimally in Polaris (NVIDIA) and Aurora (Intel)
- INCITE award used to deliver this workflow

Concept into a deliverable

Value proposition

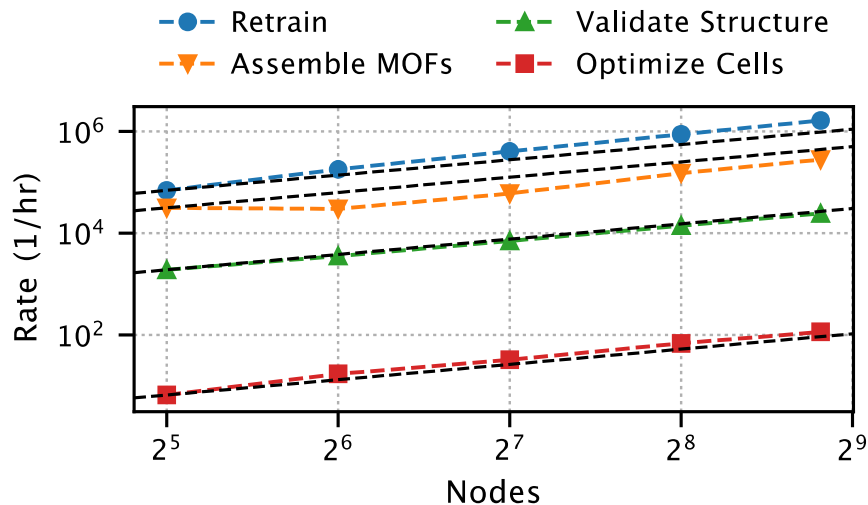
Computational and experimental science to get menu of novel materials

Accelerate discovery, synthesis and commercialization of energy materials through

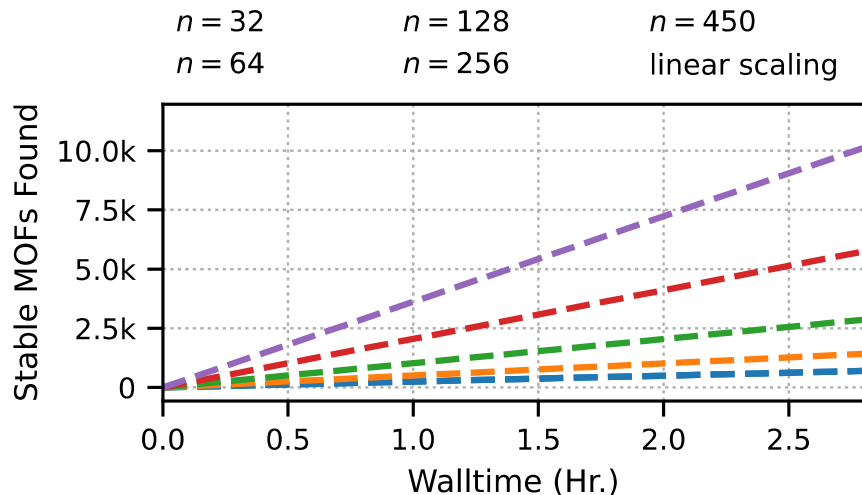
- Autonomous discovery
- Energy Storage and Conversion
- AI for Science, Energy and Security

MOFA – MATERIALS DISCOVERY AT SCALE

Yan, X., Hudson, N., Park, H., Grzenda, D., Pauloski, J. G., Schwarting, M., ... & Huerta, E. A. MOFA: Discovering Materials for Carbon Capture with a GenAI-and Simulation-Based Workflow, *arXiv:2501.10651* (2025).



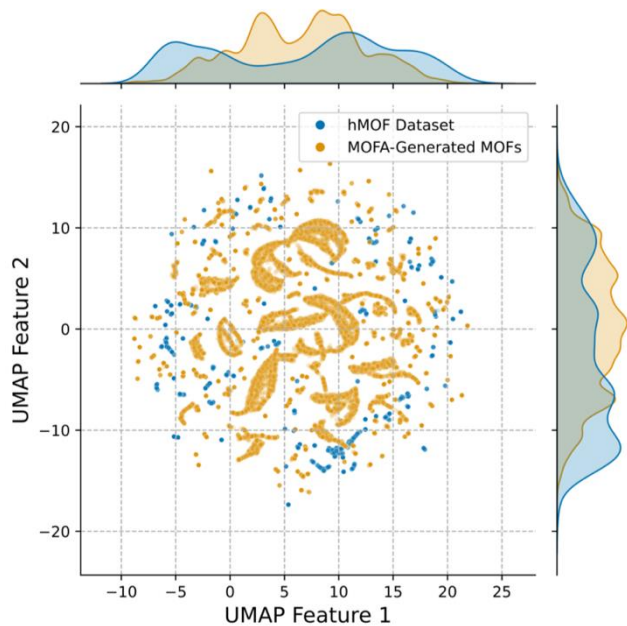
Sustained throughput in tasks per hour



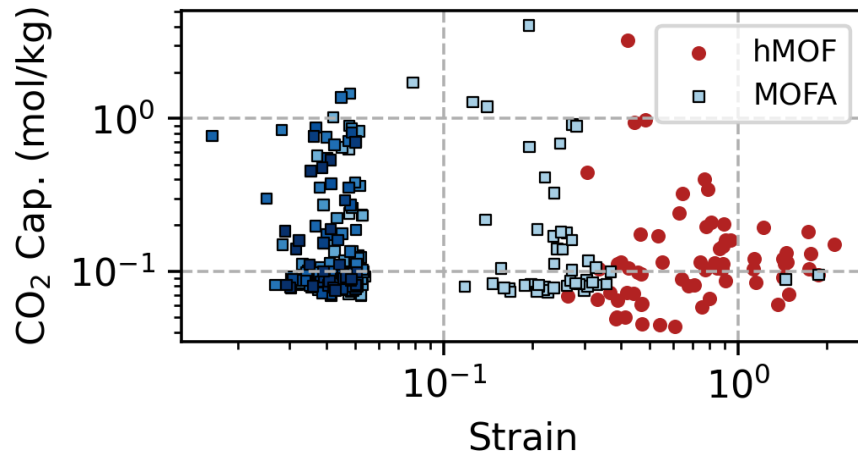
Stable MOFs found over time for MOFA runs from 32 to 450 nodes

MOFA – MATERIALS DISCOVERY AT SCALE

Yan, X., Hudson, N., Park, H., Grzenda, D., Pauloski, J. G., Schwarting, M., ... & Huerta, E. A. MOFA: Discovering Materials for Carbon Capture with a GenAI-and Simulation-Based Workflow, *arXiv:2501.10651* (2025).



Diversity of MOFA generated linkers



Storage capacity of MOFA MOFs

MOFA 2.0 – MATERIALS DISCOVERY AT SCALE

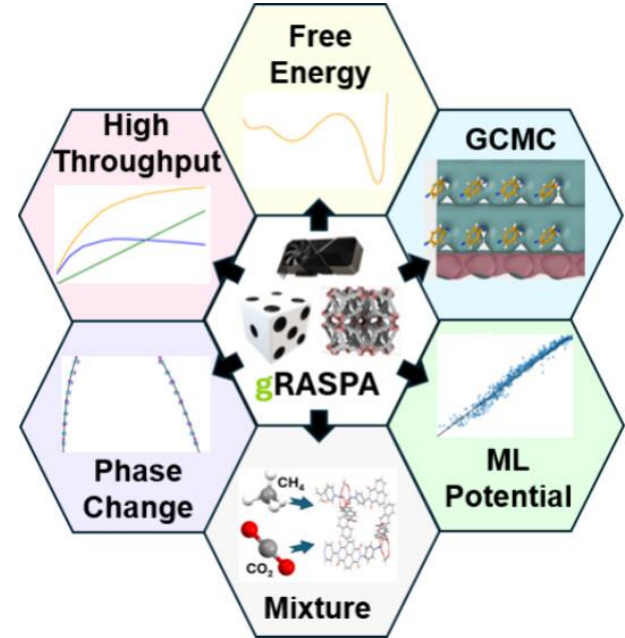
New modeling capabilities!

GPU-accelerated Monte Carlo simulation software developed by Argonne and Northwestern

Compared to RASPA2 (CPU-based software), it achieves a speedup of 8-16 times, enabling faster and more efficient modeling of adsorption and diffusion in nanoporous materials.



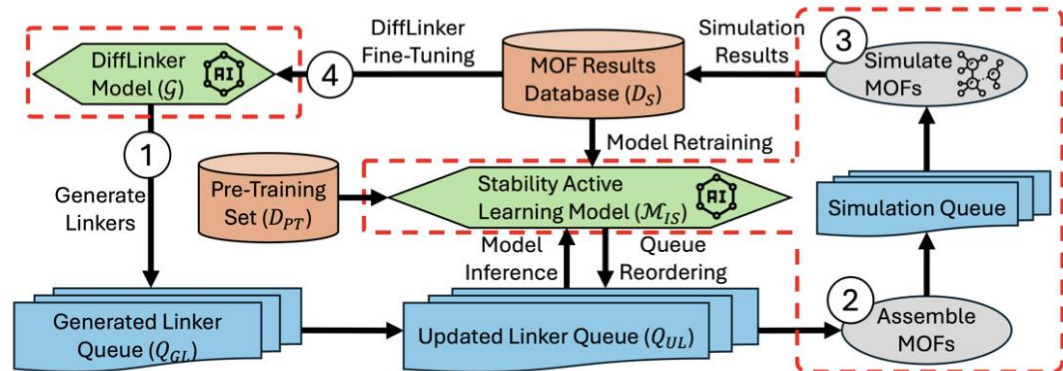
Thang Pham



AI-GUIDED QUEUE PRIORITIZATION FOR EFFICIENT MATERIALS DISCOVERY

End-to-end AI-driven MOF discovery workflow: a generative model proposes new linker molecules, candidate MOFs are assembled and evaluated with molecular dynamics simulations for structural stability, and an active-learning model continuously reorders the candidate queue to prioritize the most promising and synthesizable materials.

This closed-loop system accelerates identification of high-quality MOF candidates while minimizing expensive simulations of low-value structures.



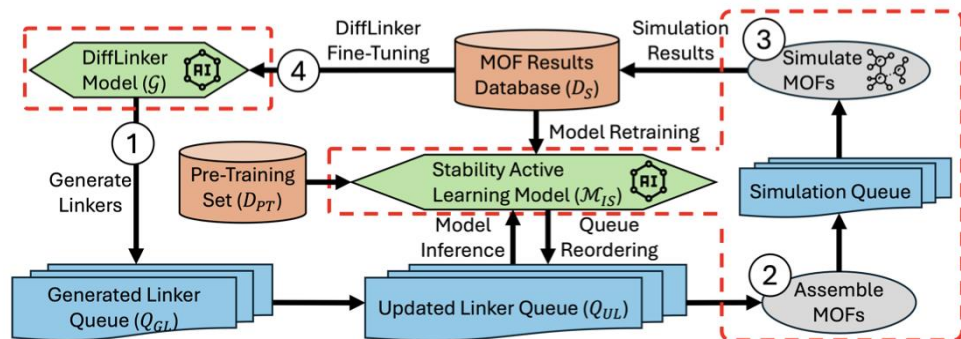
Schwartz, M., Ward, L., Hudson, N., Yan, X., Blaiszik, B., Chaudhuri, S., Huerta, E. and Foster, I. "Steering an active learning workflow towards novel materials discovery via queue prioritization." In *2025 IEEE International Conference on eScience (eScience)*, pp. 30-38. IEEE.

Best Student Paper Award at the eScience 2025 Conference!

AI-GUIDED QUEUE PRIORITIZATION FOR EFFICIENT MATERIALS DISCOVERY

Scientific Achievement

- **AI steering doubles useful discoveries.** Actively prioritizing candidates shifts computation toward viable materials, raising the fraction of high-quality discoveries from ~30% to ~60%.
- **Uncertainty-aware selection prevents model collapse.** Including exploration in the selection process avoids generative model decay and sustains long-term discovery of stable, novel materials.



Significance and Impact

- AI is shown to focus computation on viable materials instead of implausible ones, making large-scale screening far more cost-effective. The method prevents generative AI from degrading over time, allowing sustained, self-improving materials discovery at DOE scale.

Schwartz, M., Ward, L., Hudson, N., Yan, X., Blaiszik, B., Chaudhuri, S., Huerta, E. and Foster, I. "Steering an active learning workflow towards novel materials discovery via queue prioritization." In *2025 IEEE International Conference on eScience (eScience)*, pp. 30-38. IEEE.

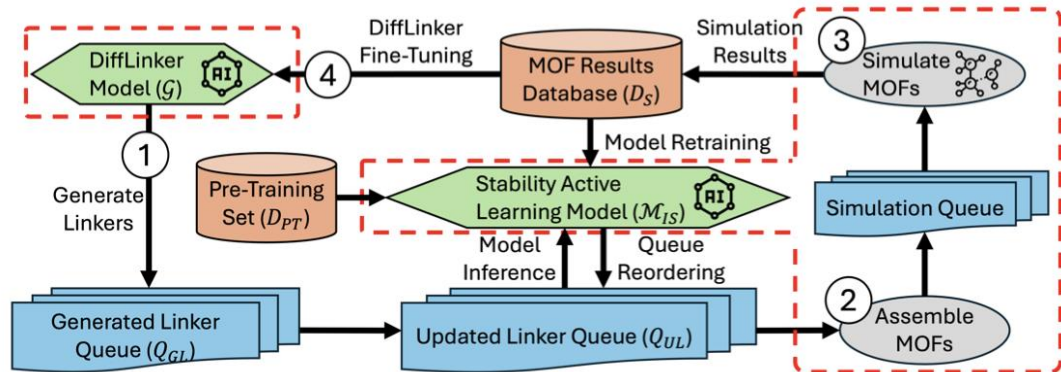
Best Student Paper Award at the eScience 2025 Conference!

AI-GUIDED QUEUE PRIORITIZATION FOR EFFICIENT MATERIALS DISCOVERY

Research Details

➤ Linked a generative AI model with an active-learning surrogate to rank and prioritize candidate materials before simulation and used molecular dynamics as the ground-truth evaluator to screen AI-generated MOFs for structural stability and viability.

➤ Evaluated exploration–exploitation strategies and measured gains in discovery rate and computational efficiency versus an unguided baseline.

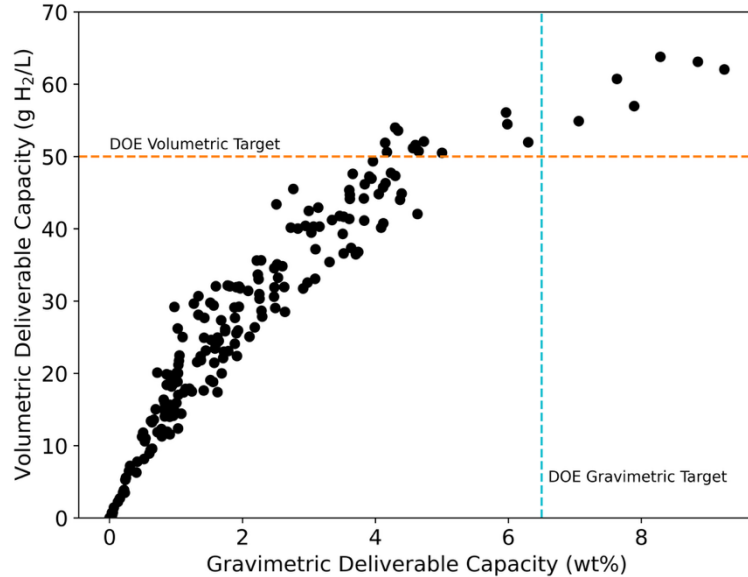


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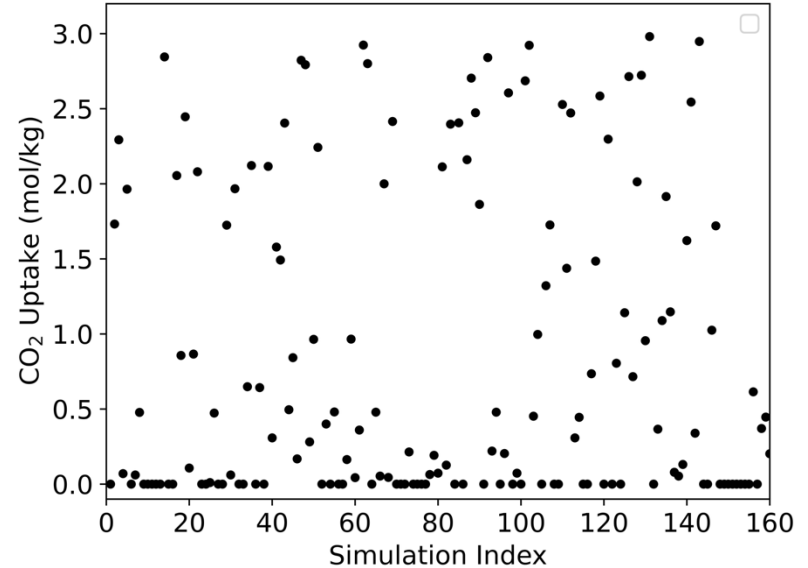
MOFA 2.0 – MATERIALS DISCOVERY AT SCALE

MOFs performance for H₂ storage and CO₂ capture from CoRE MOF database



H₂ cryogenic storage.

Deliverable capacity defined between adsorption (77K/100 bar) and desorption (160K, 5 bar)



CO₂ adsorption at 298K, 1 bar

CFD MODELING OF MOF ADSORPTION DYNAMICS

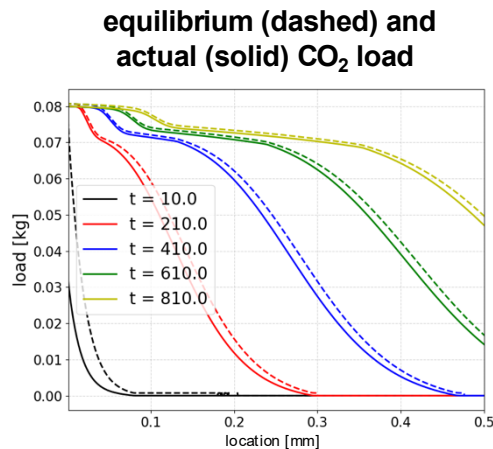
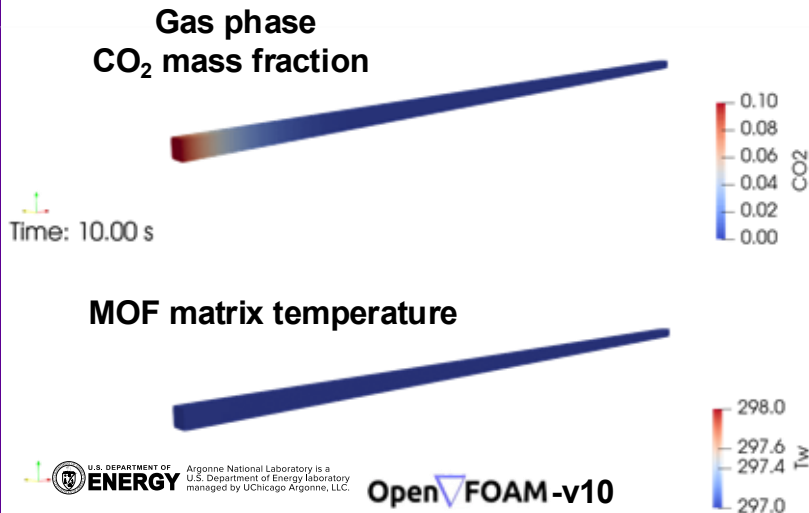
Definition of a flexible library to import AI-designed MOFs and assess their performance

Modeling approach

- Porous media modeling
- Langmuir-*like* MOF physisorption
- Species transport in gas phase
- Species diffusion in macro and micro-pores
- Heat transfer and thermal modeling of both solid and gas phase

Goals

- Assess performance of new MOFs
- Explore optimal reactor configurations (e.g., bed geometry, substrate material)
- Inform TEA/LCA workflows

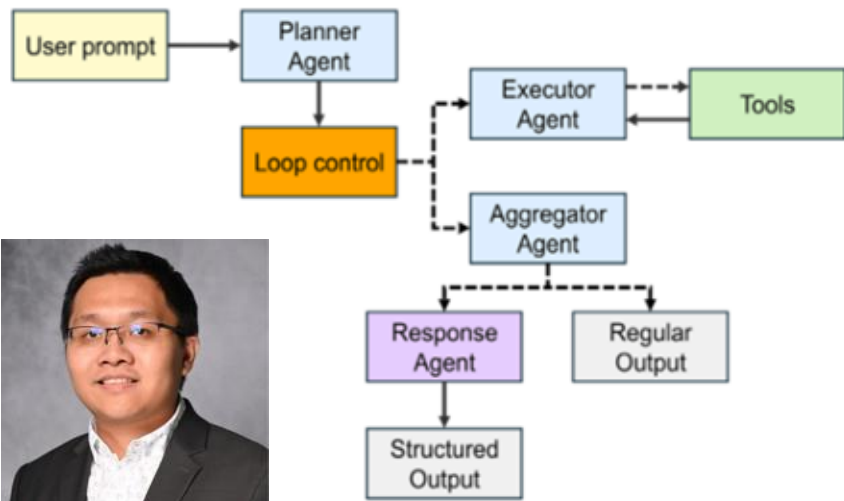


mofFOAM-10



Lorenzo Nocivelli - lnocivelli@anl.gov

INCLUDING AGENTS!



Thang Pham

Human

You are given a chemical reaction: 1 (Methane) + 2 (Oxygen) -> 1 (Carbon dioxide) + 2 (Water). Calculate the enthalpy change for this reaction using GFN2-xTB at 400K.

ChemGraph (multi-agent, GPT-4o-mini)

Planner agent

Task 1: Calculate the enthalpy of formation of methane (CH4) using GFN2-xTB at 400K
Task 2: Calculate the enthalpy of formation of oxygen (O2) using GFN2-xTB at 400K
Task 3: Calculate the enthalpy of formation of carbon dioxide (CO2) using GFN2-xTB at 400K
Task 4: Calculate the enthalpy of formation of water (H2O) using GFN2-xTB at 400K

Executor agents

Executor 1

Executor 2

Executor 3

Executor 4

Tool calls

Tool call 1: molecule_name_to_smiles(Methane)
Tool call 2: smiles_to_atomsdata("C")
Tool call 3: run_ase(Atomsdata(Methane), driver=thermo, temperature=400, "calculator"=["calculator_type": "TBLite", "method": "GFN2-xTB"])

Tool outputs

The thermochemical calculation for methane (CH4) using the GFN2-xTB method at 400K has been successfully completed [...]
Enthalpy of Formation: -112.2512 eV
[...]

[...]
Enthalpy of Formation: -214.93 eV
[...]

[...]
Enthalpy of Formation: -280.0425 eV
[...]

[...]
Enthalpy of Formation: -137.2903 eV
[...]

Aggregator agent

[...] Thus, the enthalpy change (u0394H) for the reaction is: Delta H = -12.5119 eV

Minghao Xie

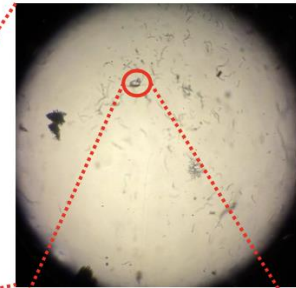


DJ Liu



**BRINGING ALL
PIECES TOGETHER**

Structural analysis of
synthesized MOFs at Argonne



Sreehari Surendran



Max Delferro



BRINGING ALL PIECES TOGETHER

Powder X-Ray Diffraction (PXRD) at scale to confirm successful MOF synthesis



Gregory K. Krumdick



BRINGING ALL PIECES TOGETHER

Scale up work at the Argonne's Materials Engineering Research Facility (MERF)



BENEFITS

**Secure energy
independence/dominance**

**Sustain U.S. production
through high-performance
materials for industry**

**Leverage economic
prosperity**



INDUSTRY

**Materials discovery and synthesis
more quickly to solve immediate
needs with national
lab expertise**

DEPARTMENT OF ENERGY

**Cost-effective materials
for upgraded efficiencies and
circular economy**

SUMMARY

CHALLENGE

The U.S. needs better mechanisms for energy storage and conversion

SOLUTION

Combine computational chemistry + AI + Exascale computers with experimental chemistry, characterization and synthesis, and cost analysis

USING ARTIFICIAL INTELLIGENCE TO ACCELERATE MATERIAL RESEARCH



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ENERGY