

Artificial Intelligence for Materials Science Workshop: Welcome and Logistics

NIST, Materials Measurement Laboratory

AIMS: July 9-10, 2025

<https://jarvis.nist.gov>



**Joint Automated Repository for Various Integrated
Simulations**

7/9/2025

Special Thank You



- Materials Genome Director: Jim Warren
- Division Chiefs: Mark VanLandingham (642), Dave Holbrook (643)
- Group Leaders: Carelyn Campbell (642), Francesca Tavazza (643)
- AIMS Co-organizers/Moderators: Daniel Wines, Kamal Choudhary, Brian DeCost, Francesca Tavazza
- NIST Conference Services: Sabina Mohan, Pauline Truong, Megan Spangler, Crissy Robinson, Carol Shibley
- NCCoE Staff
- NIST AV Team: Jonathan Mundy
- All invited speakers and participants!

Emergency Procedures for NCCoE Visitors

Evacuation Emergencies

What is an Evacuation Emergency?

- Fires
- Explosions
- Earthquakes
- Indoor toxic material releases
- Indoor radiological and biological accidents
- Workplace violence

What Will Happen During an Evacuation Event?

- A building-wide alarm will sound
- Verbal instructions over the building's public address (PA) system will follow shortly after the alarm
- Exit the conference room and head for the nearest exit (**Red Signs – Upper Right Map**)
- If the Security Guard is close by and accessible, ask for further instruction
- Once outside the building, swiftly walk toward the designated meeting area indicated on the drawing "Evacuation Meeting Area" (**Yellow notation – Lower Right Map**)

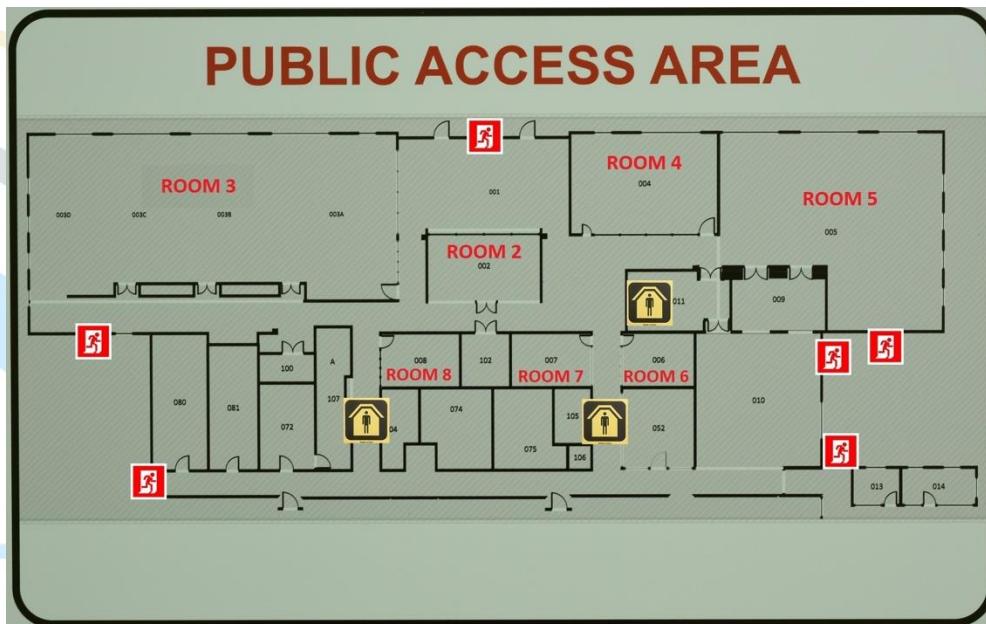
Shelter-In-Place (SIP) Emergencies

What is a Shelter-In-Place Emergency?

- Severe weather (hurricanes, tornadoes, etc.)
- chemical, biological, or radiological contaminants released into the environment

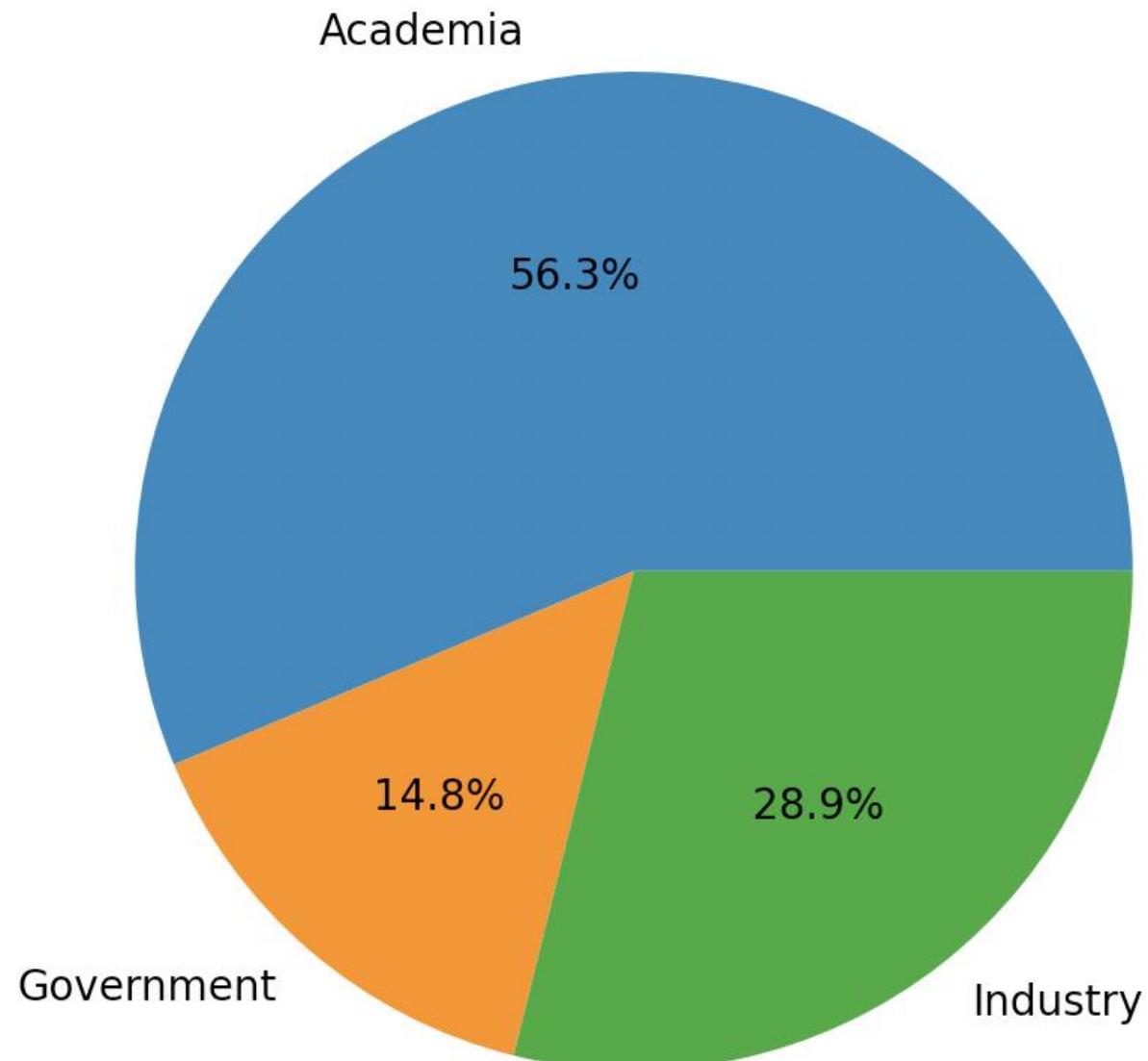
What Will Happen During an Evacuation Event?

- A building-wide alarm will sound
- Verbal instructions over the building's public address (PA) system will follow shortly after the alarm
- Exit the conference room and head for the nearest SIP hallway or room (**Yellow Signs – Upper Right Map**)
- If the Security Guard is close by and accessible, ask for further instruction



Welcome to AIMS 2025!

NIST



Registered: 143
Speakers: 22
Posters: 31

Agenda: Day 1



*All invited talks will be 20 minutes, including time for questions

Day 1: July 9						
Session I: 9:00-12:00		Lunch: 12:00-1:00	Session 2: 1:00-3:20		Panel Discussion 3:20 - 4:00	Poster Session: 4:00 - 5:30
Opening Remarks: Jim Warren	9:00-9:10		Benji Maruyama	1:00-1:20	Tess Smidt	
Overview and Logistics: Daniel Wines	9:10-9:25		Ichiro Takeuchi	1:20-1:40	Olga S. Ovchinnikova	
Arun Mannodi-Kanakkithodi	9:25-9:45		Panchapakesan Ganesh	1:40-2:00	Joseph Krause	
Ankit Agrawal	9:45-10:05		Break	2:00-2:20	Benji Maruyama	
Olexandr Isayev	10:05-10:25		Joseph Krause	2:20-2:40	Ali Hamze	
Break: Group Picture	10:25-10:45		Jiaman Hu	2:40-3:00		
Simon J.L. Billinge	10:45-11:05		Olga S. Ovchinnikova	3:00-3:20		
Roberto Car	11:05-11:25					
Tess Smidt	11:25-11:45					

Agenda: Day 2



Day 2: July 10				
Session 3: 9:00-12:00		Lunch: 12:00-1:00	Session 4: 1:00-2:20	Hands On Session: 2:15 - 4:30
			Milad Abolhasani 1:00-1:20	
Heather Kulik 9:05- 9:25			Shengyen Li 1:20-1:40	
Aditya Nandy 9:25- 9:45			Nathan Johnson 1:40-2:00	
Corey Oses 9:45- 10:05				
Break 10:05- 10:25				
Ali Hamze 10:25- 10:45				
Brandon Wood 10:45- 11:05				
Luis Barroso-Luque 11:05- 11:25				
Steven Torrisi 11:25- 11:45				

*All invited talks will be 20 minutes, including time for questions⁶

Hotel Shuttle Schedule



Wednesday, July 9

Hotel to NCCoE:
7:45am, 8:15am and 8:30am

NCCoE back to hotel:
4:15pm, 5:15pm & 5:30pm

Thursday, July 9

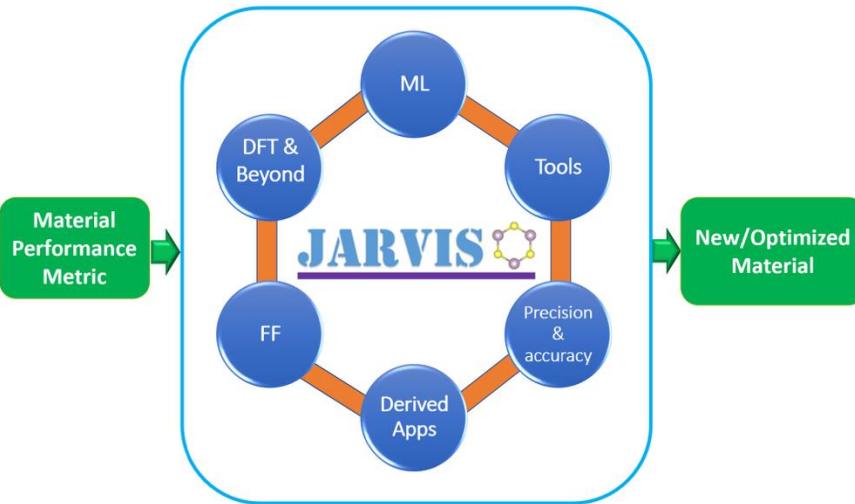
Hotel to NCCoE:
7:45am, 8:15am and 8:30am

NCCoe back to hotel:
2:30pm, 3:30 & 4:15pm

JARVIS: Databases, Tools, Events, Outreach



<https://jarvis.nist.gov>



A screenshot of the JARVIS website's "Resources" section. It displays several cards for different tools and databases:

- Density functional theory (JARVIS-DFT)
- Force-field (JARVIS-FF)
- JARVIS-QETB
- JARVIS-ALIGNN
- JARVIS-ML
- Machine learning (CFID)
- JARVIS-WannierTB
- JARVIS-Tutorials
- Databases

Established: January 2017

Published: >50 articles

Users: >150,000+ users worldwide

Materials: >80000, millions of properties

Events:

- Quantum Matters in Materials Science (QMMS)
- Artificial Intelligence for Materials Science (AIMS) **[July 9-10, 2025]**
- JARVIS-School **(reach out if interested)**



usnistgov / jarvis

User-comments:

- “There are many different theoretical levels on which you can approach the field. JARVIS is unusual in that it spans more levels than other databases.”
- “A pure gold-mine for the data-quality effort...”
- Thanks for your generous sharing. Your works inspire me a lot.
- “You guys are doing something really beneficial...”
- “I find JARVIS-DFT very useful for my research...”

Starred 328

downloads 647k

[Choudhary et al., npj Computational Materials 6, 173 \(2020\).](#)
[Wines et al., Applied Physics Reviews 10, 041302 \(2023\).](#)

JARVIS-DFT Website

NIST

jarvis.nist.gov/jarvisdft/

NIST

JARVIS Publications Colab Downloads Tutorials Events Log In / Sign Up Help

Density Functional Theory (DFT)

Click on periodic table elements (e.g., Ni-Al-) or enter a chemical formula (e.g., Al₂O₃) or enter a JARVIS-ID (e.g., JVASP-1002) and click Search.

Mo-S-

Search Refresh

https://jarvis.nist.gov/jarvisdft

Search:

Visualizing Atomic structure

JARVIS API JARVIS-DFT JARVIS-ML JARVIS-FF JARVIS-Tools Documentation Publications Report bug/Contact

Structure XRD DOS Bands Spillage Optics(GGA) Elastic Thermoelectric Convergence

ID: JVASP-664	Functional: OptB88vdW	Primitive cell	Primitive cell	Conventional cell	Conventional cell
Chemical formula: MoS ₂	Formation energy/atom (eV): -0.88454	a 3.19 Å	α : 90.0°	a 3.19 Å	α : 90.0°
Space-group:P-6m2 (187)	Relaxed energy/atom (eV): -5.21029	b 3.19 Å	β : 90.0°	b 3.19 Å	β : 90.0°
Crystal system:hexagonal	Point group:-6m2	c 34.88 Å	γ : 120.0°	c 34.88 Å	γ : 120.0°
Data source:JARVIS-DFT-VASP	Material type:SingleLayer	Density (g/cm ³): 0.665	Volume (Å ³): 306.988	nAtoms_prim: 3	nAtoms_conv: 3
SCF direct bandgap (eV): 1.683	SCF indirect bandgap (eV): 1.658	Magnetic moment (μ_B): 0.0	Exfoliation energy (meV/atom):	Packing fraction: 0.089	Number of species: 2
Band direct gap (eV): 1.71	Band indirect gap (eV): 1.71	TBmBJ direct gap (eV):	TBmBJ indirect gap (eV):	HSE06 direct gap (eV): 2.49	HSE06 indirect gap (eV): 2.36
Voigt bulk mod. (GPa):	Voigt shear mod. (GPa):	Poisson ratio:	Anisotropy ratio:	Solar SLME (%):	Solar SQ (%):
Max. IR mode (cm ⁻¹):	Max. Raman mode (cm ⁻¹):	Min. IR mode (cm ⁻¹):	Min. FD phonon (cm ⁻¹):	Cut-off (eV): 550	K-point length (Å): 25

Show POSCAR Show POSCAR-conv Show XYZ format Show CIF format

Visualizing Atomic structure

JARVIS-DFT



Features	JARVIS-DFT	Features	JARVIS-DFT
#Materials (Struct., E _f , E _g)	80000	2D monolayers	1011
DFT functional/methods	vdW-DFT-OptB88, TBmBJ, DFT+SOC	Raman spectra	400
K-point/cut-off	Converged for each material	Seebeck, Power Factors	23210
SCF convergence criteria	Energy & Forces	Solar SLME	8614
Elastic tensors & point phonons	17402	Spin-orbit Coupling Spillage	11383
Piezoelectric, IR spect.	4801	WannierTB	1771
Dielectric tensors (w/o ion)	4801 (15860)	STM images	1432
Electric field gradients	11865	Surfaces	300
SuperCon T _c	2200 (1058 ambient condition)	Defects	400
		Interfaces	1.4 trillion (IU), 600 (ASJ)

US CHIPS Act

- Awarded \$5.2 million over 4 years
- Project: Multiscale Modeling and Validation of Semiconductor Materials and Devices

US CHIPS Act 2022, \$52 billion



JARVIS is a repository for standardizing computational tools for materials modeling including force fields (FF) and ML for density functional theory (DFT). JARVIS has over 6,000 users and 300,000 downloads. For more information: jarvis.nist.gov

Recent Updates to JARVIS

NIST

Applied Physics Reviews

REVIEW

pubs.aip.org/aip/are

Recent progress in the JARVIS infrastructure for next-generation data-driven materials design

Cite as: Appl. Phys. Rev. **10**, 041302 (2023); doi: [10.1063/5.0159299](https://doi.org/10.1063/5.0159299)

Submitted: 22 May 2023 · Accepted: 18 September 2023 ·

Published Online: 18 October 2023



Daniel Wines,¹ Ramya Gurunathan,¹ Kevin F. Garrity,¹ Brian DeCost,¹ Adam J. Biacchi,² Francesca Tavazza,¹ and Kamal Choudhary^{1,a)}

AFFILIATIONS

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²Physical Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA

Article | [Open access](#) | Published: 15 November 2021

Atomistic Line Graph Neural Network for improved materials property predictions

[Kamal Choudhary](#) & [Brian DeCost](#)

[npj Computational Materials](#) **7**, Article number: 185 (2021) | [Cite this article](#)

25k Accesses | 210 Citations | 27 Altmetric | [Metrics](#)

Digital Discovery

PAPER



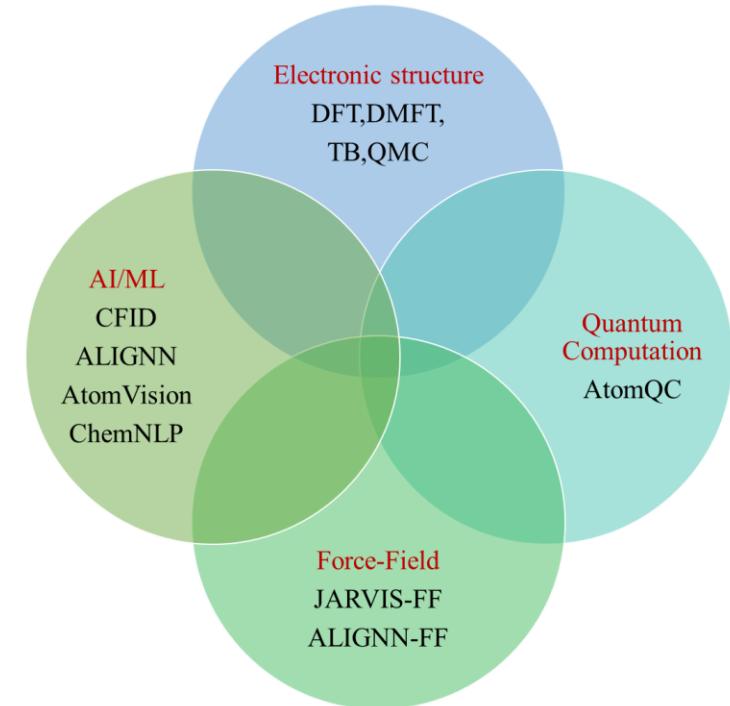
Cite this: DOI: [10.1039/d2dd00096b](https://doi.org/10.1039/d2dd00096b)



[View Article Online](#)
[View Journal](#)

Unified graph neural network force-field for the periodic table: solid state applications

Kamal Choudhary, ^{*ab} Brian DeCost, ^c Lily Major, ^{de} Keith Butler, ^e Jeyan Thiyagalingam ^e and Francesca Tavazza ^c



CHIPS-FF: Evaluating Universal MLFFs



www.acsmaterialsletters.org

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CHIPS-FF: Evaluating Universal Machine Learning Force Fields for Material Properties

Published as part of ACS Materials Letters special issue "Machine Learning for Materials Chemistry".

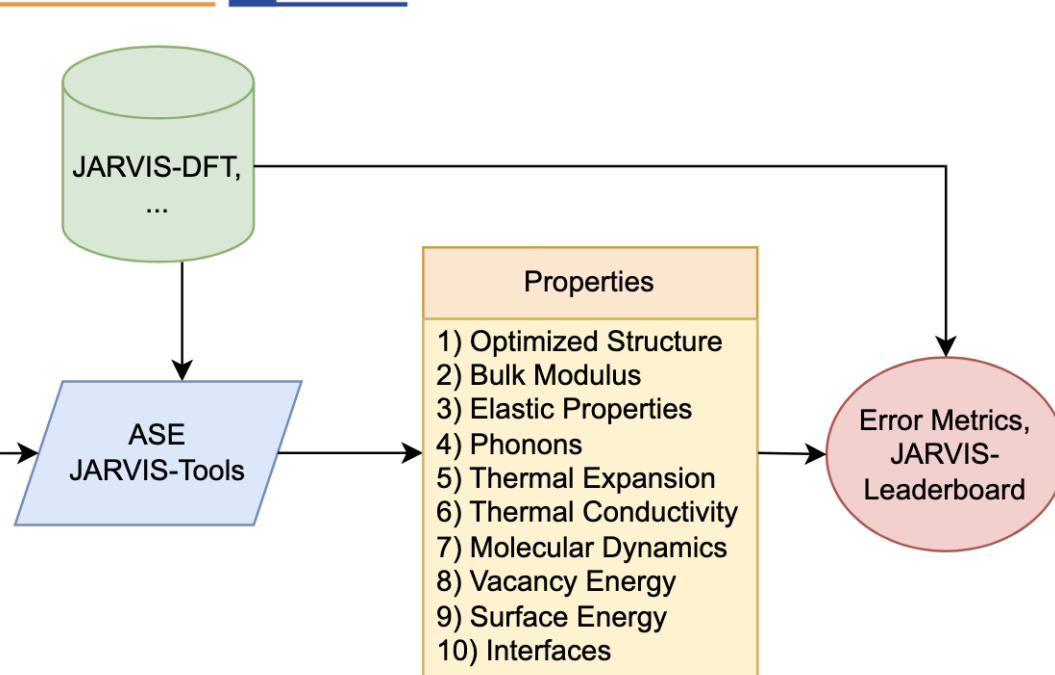
Daniel Wines* and Kamal Choudhary

Cite This: ACS Materials Lett. 2025, 7, 2105–2114

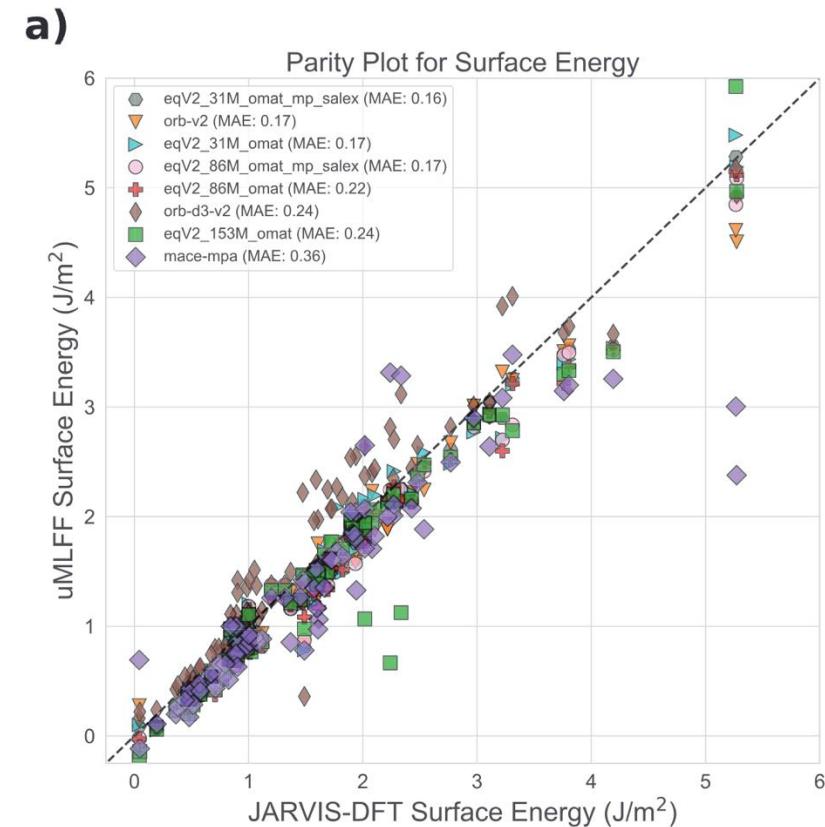
Read Online

CHIPS-FF

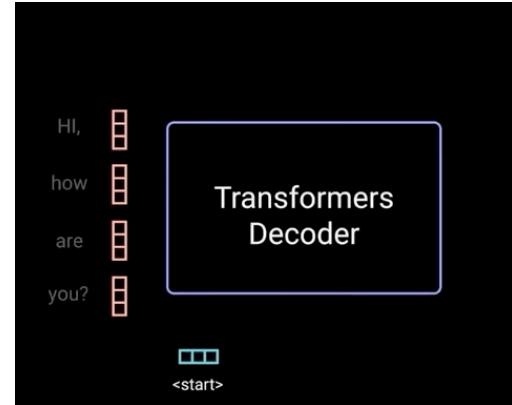
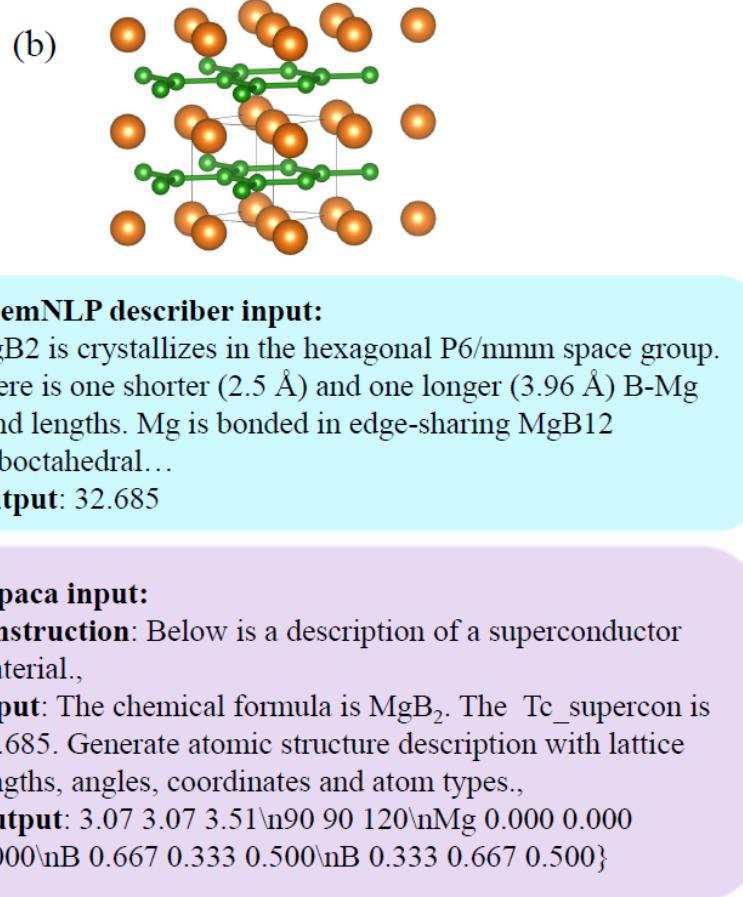
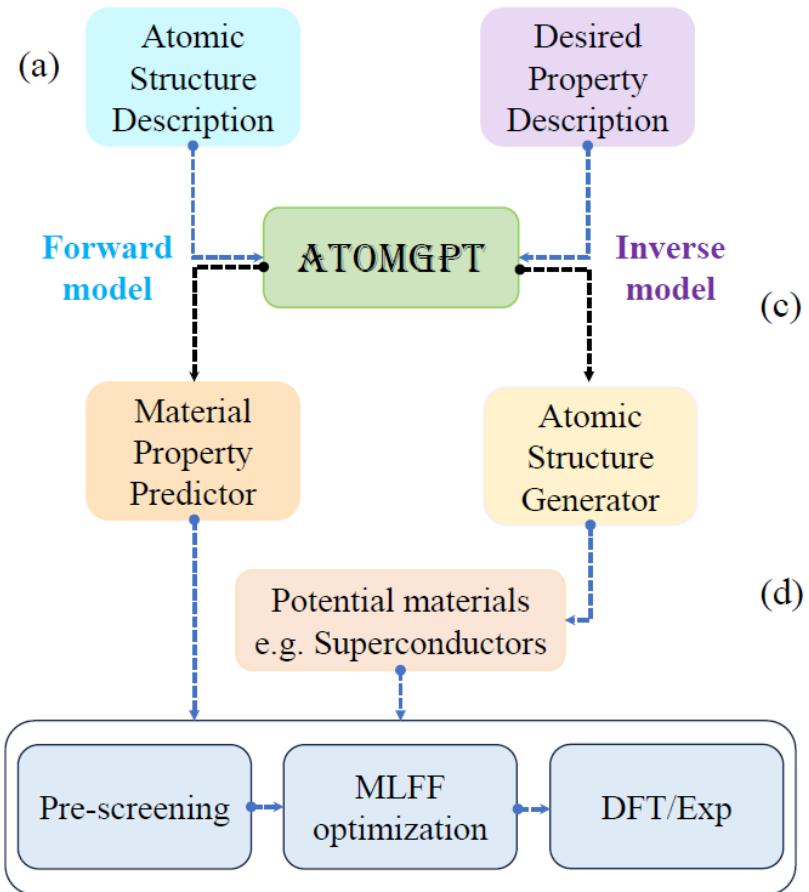
Universal MLFFs
1) MatGL
2) CHGNet
3) ALIGNN-FF
4) MACE
5) SevenNet
6) ORB
7) eqV2
8) MatterSim



<https://github.com/usnistgov/chipsff>



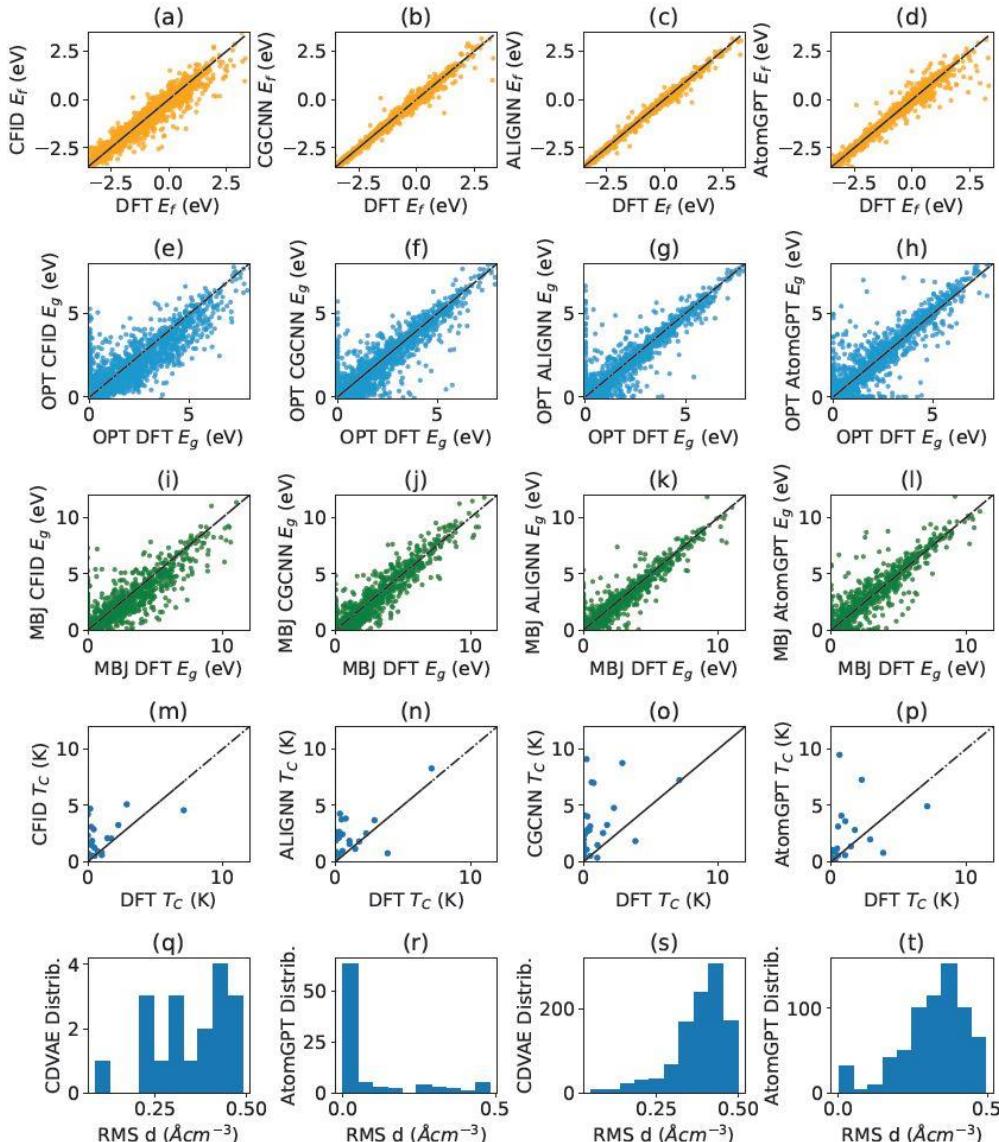
AtomGPT



$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$



- HuggingFace ecosystem
- Modified language model head for forward models
- Low-rank adaptation (LoRA) for parameter-efficient fine-tuning (PEFT)
- Rotary position embedding (RoPE)
- Transformer reinforcement learning (TRL)



	Forward models			
Prop/MAE	CFID	CGCNN	ALIGNN	AtomGPT
E_{form} (eV/atom)	0.142	0.063	0.033	0.072
OPT E_g (eV)	0.299	0.199	0.142	0.139
MBJ E_g (eV)	0.531	0.407	0.310	0.319
T_C (K)	1.99	2.60	2.03	1.54
	Inverse models			
Database/RMSE	CDVAE	AtomGPT		
SuperConDB	0.24	0.08		
Carbon24	0.36	0.32		

AtomGPT: Atomistic Generative Pretrained Transformer for Forward and Inverse Materials Design

Kamal Choudhary*

Cite this: *J. Phys. Chem. Lett.* 2024, 15, XXX, 6909–6917

Publication Date: June 27, 2024

<https://doi.org/10.1021/acs.jpclett.4c01126>

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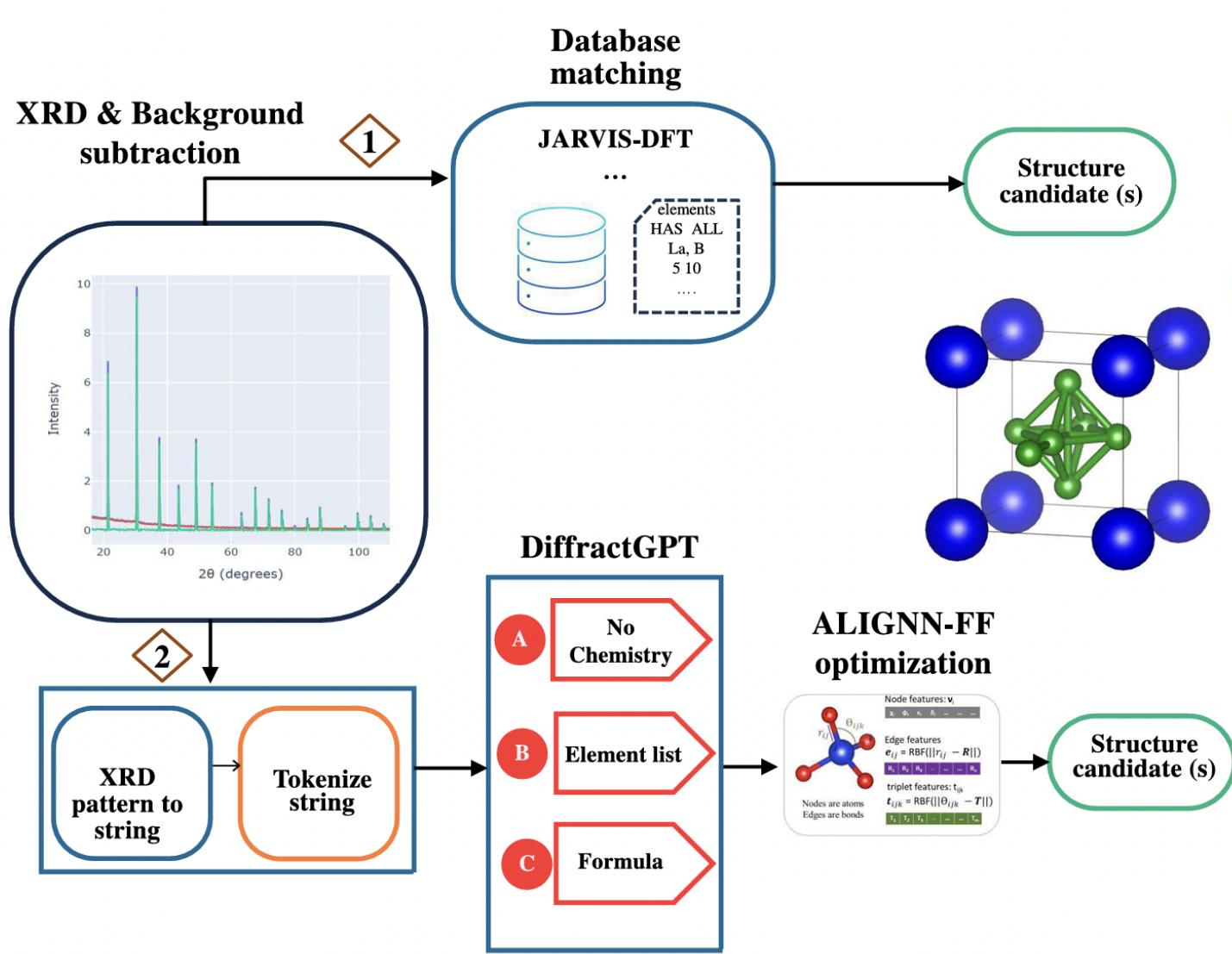
Altmetric

Citations

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DiffractGPT



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LETTERS

A JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

pubs.acs.org/JPCL

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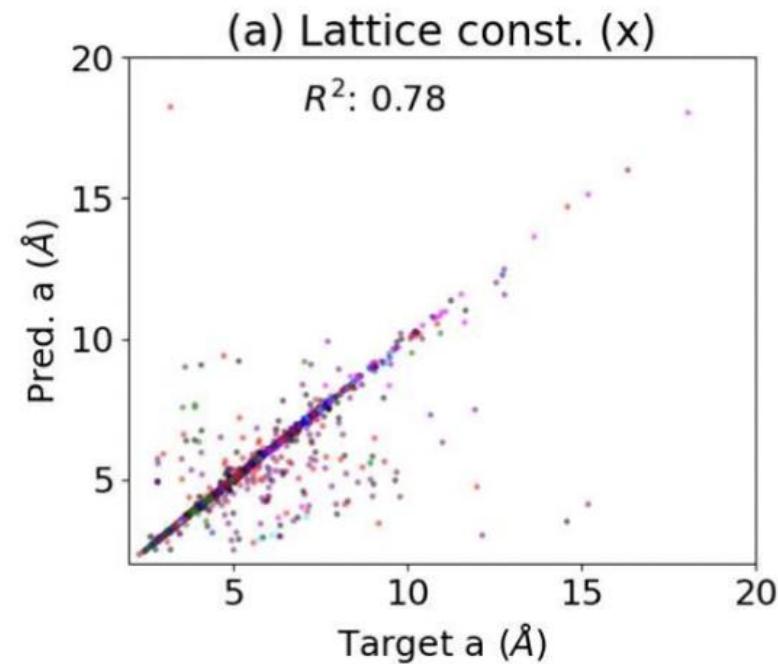
Letter

DiffractGPT: Atomic Structure Determination from X-ray Diffraction Patterns Using a Generative Pretrained Transformer

Kamal Choudhary*

Cite This: *J. Phys. Chem. Lett.* 2025, 16, 2110–2119

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MicroscopyGPT



THE JOURNAL OF
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MicroscopyGPT: Generating Atomic-Structure Captions from Microscopy Images of 2D Materials with Vision-Language Transformers

Kamal Choudhary*

Cite This: *J. Phys. Chem. Lett.* 2025, 16, 7028–7035

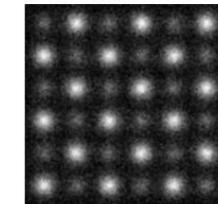
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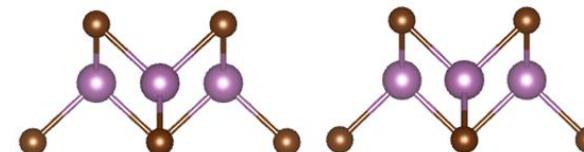
Open Access

Letter

(a) STEM image

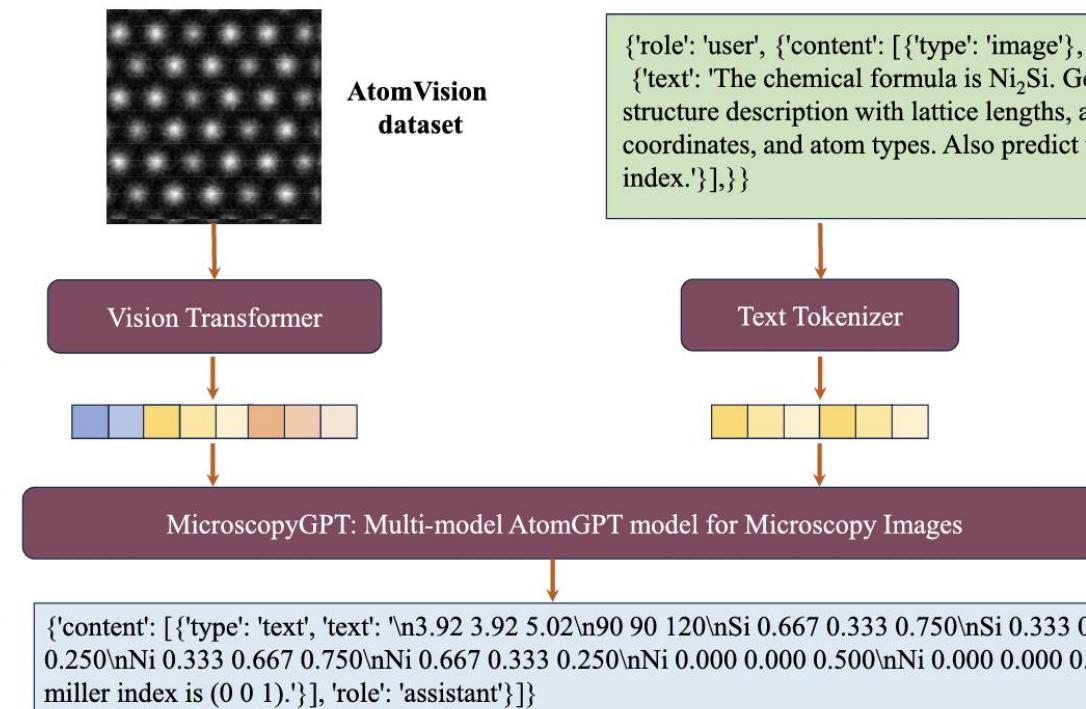
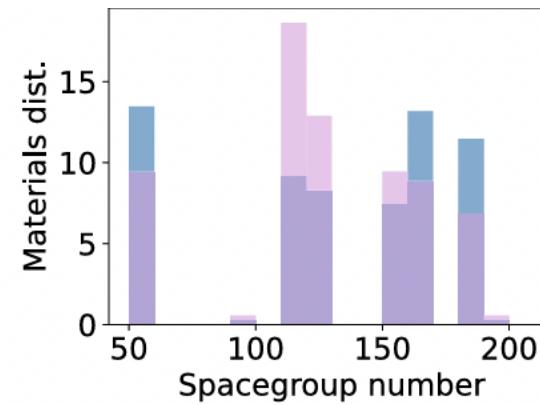
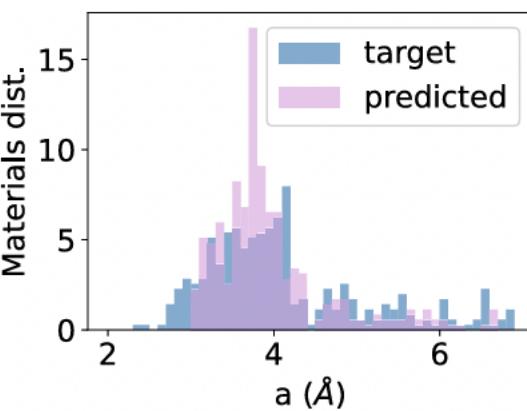


(b) Target



(c) Predicted

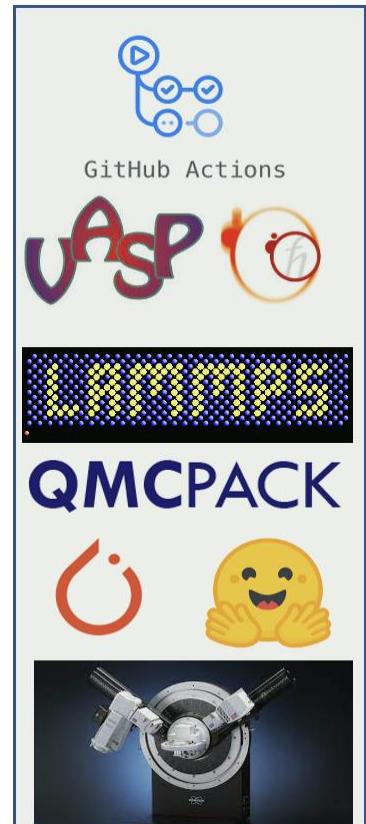
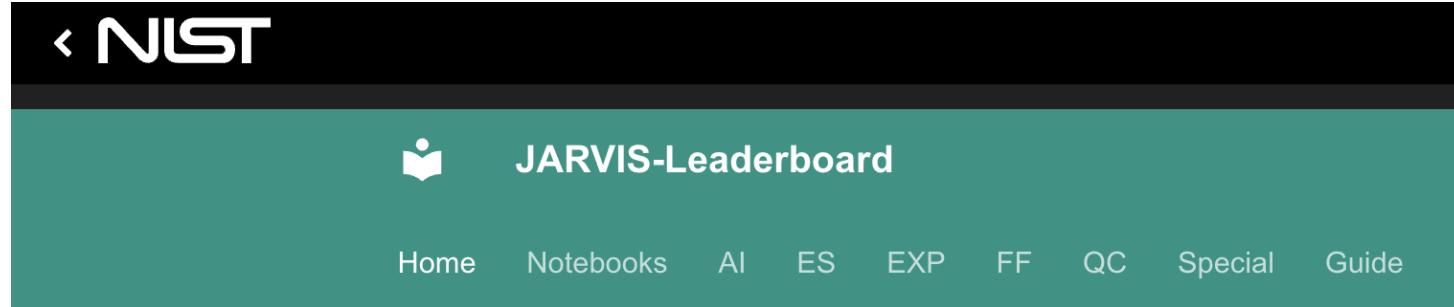
ScBr (P4/nmm)
RMSE: 0.003



JARVIS-Leaderboard: Large Scale Benchmark

Challenges in materials science community:

- Reproducibility
- Transparency
- Validation
- Fidelity
- Data vs. metadata
- What is the ground truth/reference to compare our models to? How does this change depend on the model?
- Synergy of computational and experimental databases



https://pages.nist.gov/jarvis_leaderboard/

Community effort to tackle challenges:

A screenshot of a Nature journal article page. The URL in the address bar is nature.com/articles/s41524-024-01259-w. The page title is "JARVIS-Leaderboard: a large scale benchmark of materials design methods". The authors listed are Kamal Choudhary, Daniel Wines, Kangming Li, Kevin F. Garrity, Vishu Gupta, Aldo H. Romero, Jaron T. Krogel, Kayahan Saritas, Addis Fuhr, Panchapakesan Ganesh, Paul R. C. Kent, Keqiang Yan, Yuchao Lin, Shuiwang Ji, Ben Blaiszik, Patrick Reiser, Pascal Friederich, Ankit Agrawal, Pratyush Tiwary, Eric Beyerle, Peter Minch, Trevor David Rhone, Ichiro Takeuchi, Robert B. Wexler, ... Francesca Tavazza. There is a "Show authors" link at the bottom right.

Categories of benchmarks

Explore State-of-the-Art Materials Design Methods

Artificial intelligence
(AI)

Contributions: 1034

[See All Benchmarks](#)

Electronic Struct.
(ES)

Contributions: 741

[See All Benchmarks](#)

Force-field
(FF)/potentials

Contributions 282

[See All Benchmarks](#)

Quantum Comput.
(QC)

Contributions: 6

[See All Benchmarks](#)

Experiments (EXP)

Contributions: 25

[See All Benchmarks](#)

Example Notebooks

Notebooks: 16

[See All Notebooks](#)

Methodologies

Available Methods: 503

[Learn more](#)

Contribution Guide

Contributors: 26

[Learn more](#)

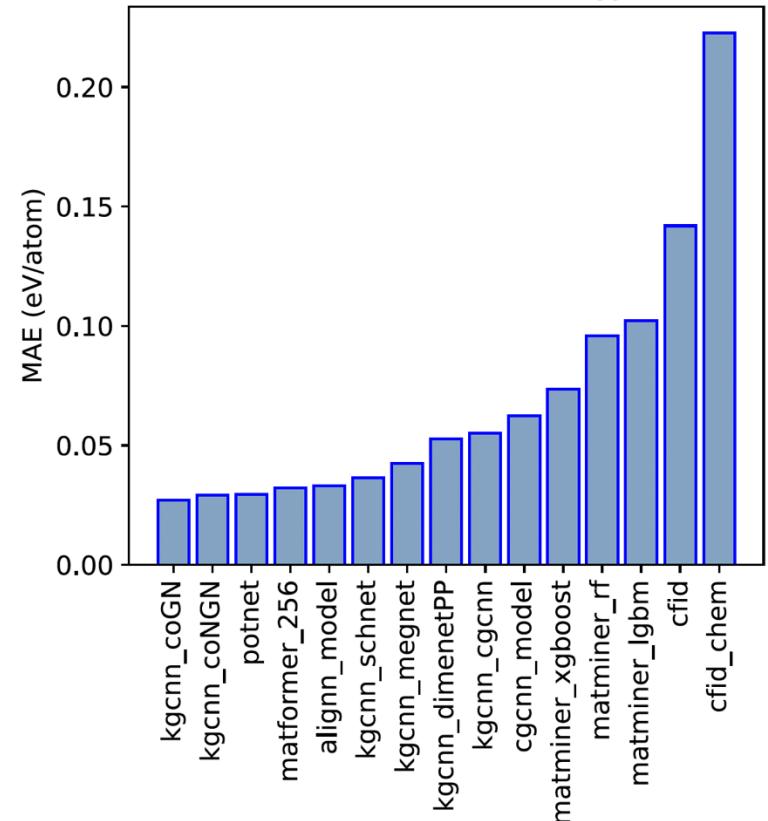


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U.S. Department of Commerce



- 1) Electronic Structure
- 2) Artificial Intelligence
- 3) Force Field
- 4) Quantum Computation
- 5) Experiment

(a) AI (formation energy)

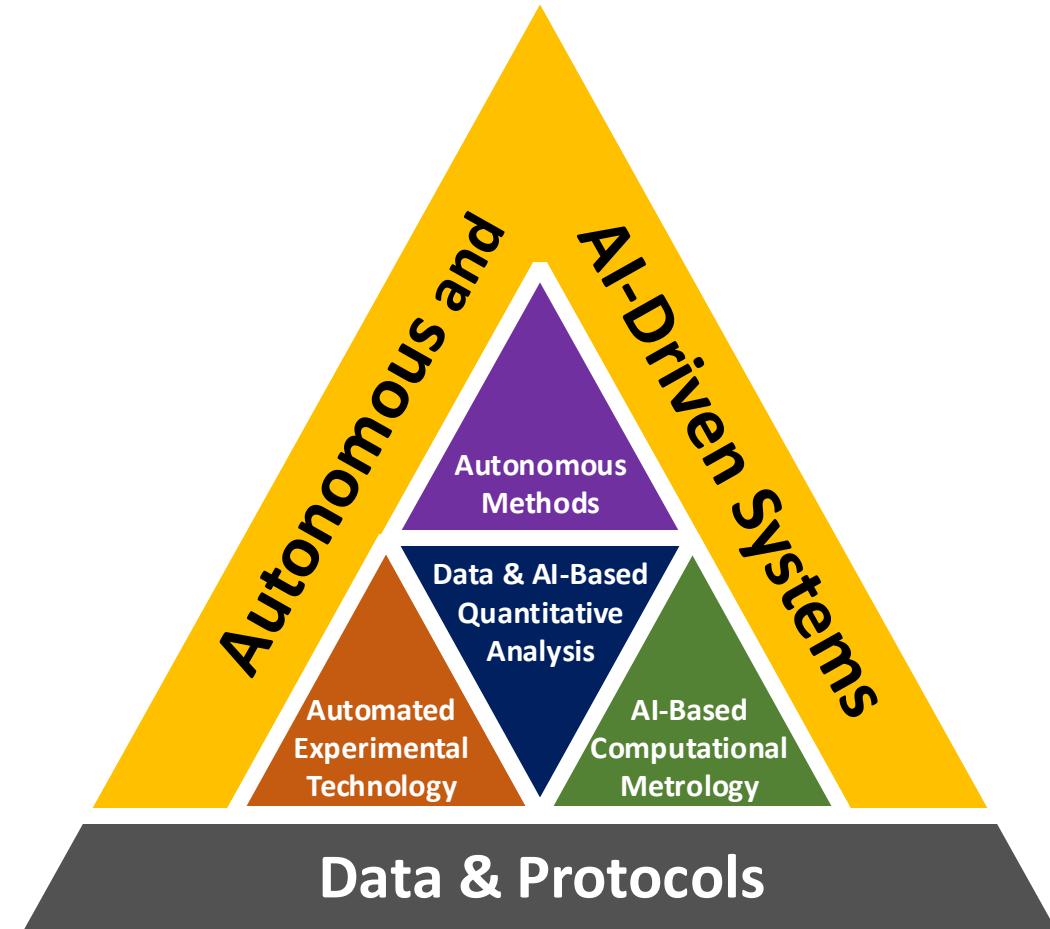


Data and AI-Driven Materials Science Group

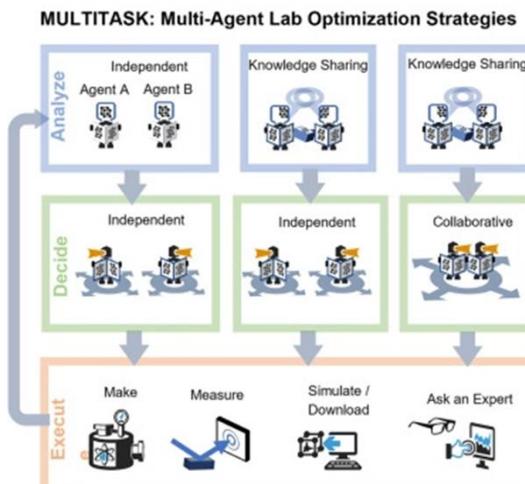
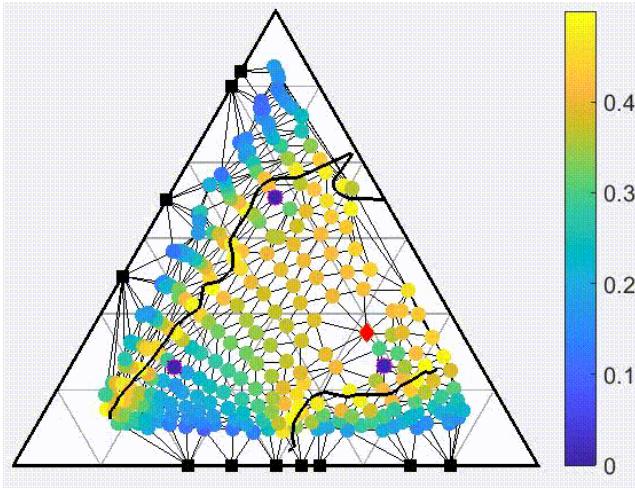
Autonomous and AI-Driven Systems — Developing Autonomous Methods that form the **core decision-making capability of self-driving laboratories**, as well as **robust automated Data and AI-Based Quantitative Analysis**.

- **Autonomous Methods** — methods development to support autonomous execution of: **materials synthesis and characterization, simulation execution, data management, cleaning, analysis and interpretation, model and knowledge generation, and decision making.**
- **Data and AI-Based Quantitative Analysis** — we combine physical models with a range of modern statistical methods to replace non-repeatable human biases with **traceable and specified algorithmic approaches for data analysis.**
- **Automated Experimental Technology** — Development of **automated, robotic, and high-throughput experimental infrastructure** to accelerate the generation of reproducible and trustworthy experimental data.
- **AI-Based Computational Metrology** — Development of machine learning systems to accelerate and scale up physics-based modeling and simulation.

Data and Protocols — Development of protocols for **interoperable laboratory infrastructure, materials traceability, and FAIR materials data.**



Projects



❖ Autonomous Methods:

- CAMEO: Closed-loop autonomous materials exploration and optimization
- ANDiE: Autonomous Neutron Diffraction Explorer
- MULTITASK: MULTI-agent auTonomous fAcilities - a Scalable frameworkK

❖ Data and AI-Based Quantitative Analysis:

- Automated model fitting for electrochemical corrosion assays
- Automated structural phase identification from x-ray diffraction
- High throughput quantitative x-ray diffraction analysis
- EXAFS analysis with focus on characterization of short range order in alloys

❖ Automated Experimental Technology:

- High Throughput Combinatorial Synthesis
- Autonomous Scanning Droplet Cell

❖ AI-Based Computational Metrology:

- ML algorithm development and AI Benchmarking
- Performance Metrics for Direct Air Capture of Carbon Dioxide

❖ Data and Protocols:

- FAIR Digital Object Framework
- EV Battery Passport

Acknowledgement and Collaboration

NIST
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U.S. Department of Commerce



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(NIST, 643)

