

5th Artificial Intelligence for Materials Science Workshop: Welcome and Logistics

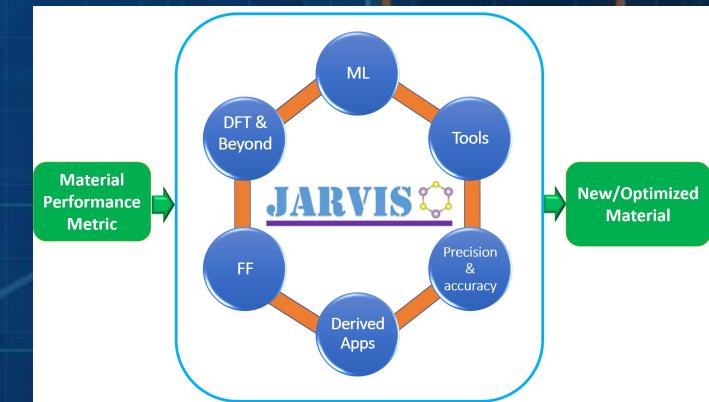


Kamal Choudhary

NIST, Gaithersburg, MD, USA
AIMS: July 17-18, 2024

Estd. 1901

Joint Automated Repository for Various Integrated Simulations



<https://jarvis.nist.gov>

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, Kevin Garrity, Brian DeCost, Austin McDannald, Howie Joress, and Francesca Tavazza
- NIST Conference Services: Sabina Mohan, Terri Viezbicke, Jennifer Gerlock, Timothy Czakoczi and 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**)

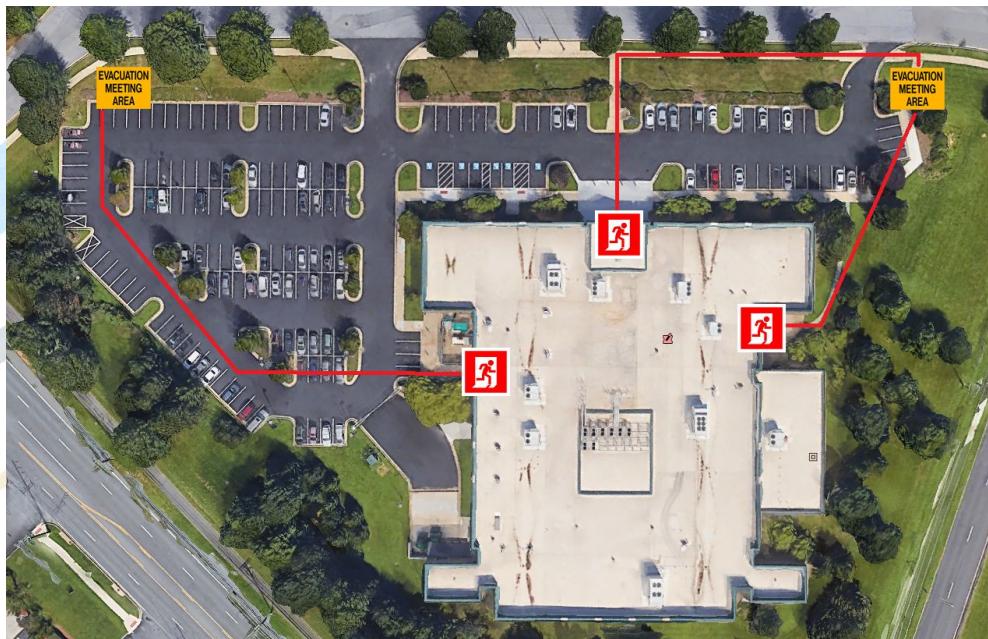
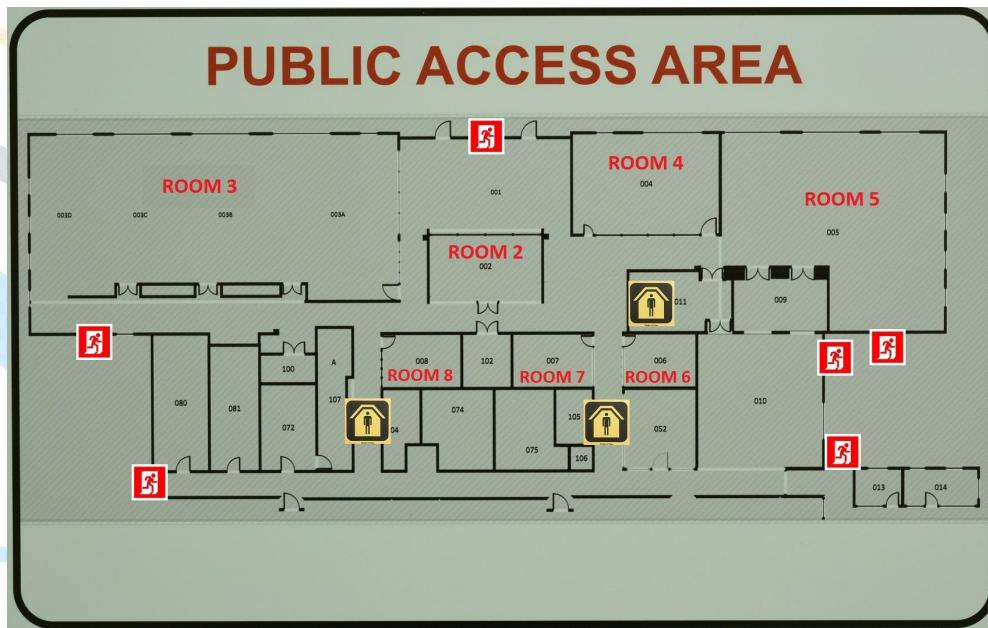
Shelter-In-Place (SIP) Emergencies

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?

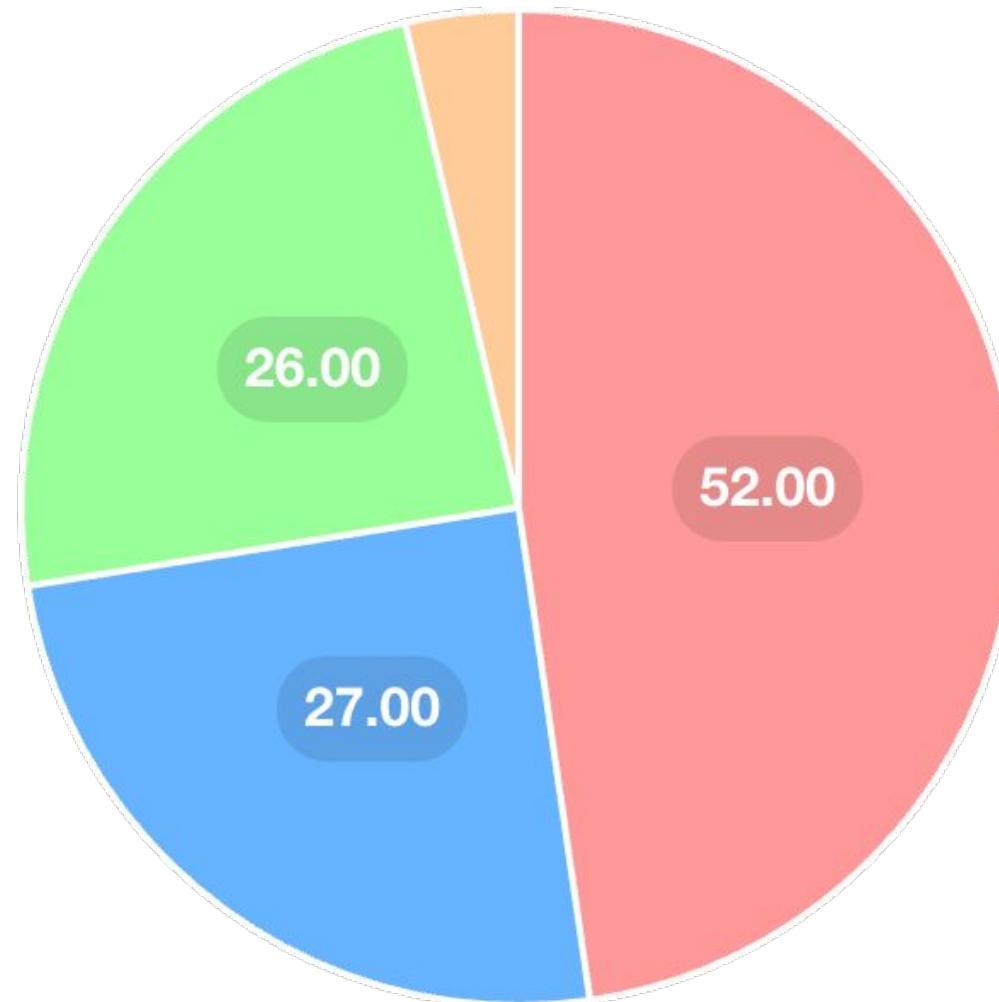
- A building-wide alarm will sound
- Verbal instructions over the building's public address (PA) system will follow shortly after the alarm
- Exit the conference room and head for the nearest SIP hallway or room (**Yellow Signs – Upper Right Map**)
- If the Security Guard is close by and accessible,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



Welcome to AIMS 2024!

NIST

For ■ Academia, ■ Government, ■ Industry, and ■ Other



Registered: 109

Students: 25

Postdocs: 10

Agenda: Day 1

DATE: Day 1				
Start Time	End Time	Speaker(s)	Session Name/Information	AV/CS Notes:
9:00	9:10	Jim Warren	Opening remarks by Jim Warren	
9:10	9:25	Kamal Choudhary	Overview and Logistics	
9:25	11:45	Nicola Marzari (9:25-9:45) <ul style="list-style-type: none"> Machine learning electrochemistry P. Ganesh, Abdulgani Annaberdiyev (9:45-10:05) <ul style="list-style-type: none"> Predicting Quantum Monte Carlo Charge Densities using Graph Neural Networks Anouar Benali (10:05-10:25) <ul style="list-style-type: none"> Increasing AI/ML Predictions Through DMC-enhanced Delta Learning Break (10:25-10:45) Ming Hu (10:45-11:05) <ul style="list-style-type: none"> Unleashing the Power of Artificial Intelligence for Phonon Thermal Transport Christopher Sutton (11:05-11:25) <ul style="list-style-type: none"> Machine learning models for accelerating materials discovery Hongliang Xin (11:25-11:45) <ul style="list-style-type: none"> Accelerating Scientific Discovery in Catalysis with Artificial Intelligence 	Invited Session I Chair: Daniel Wines	
12:00	1:00		Lunch	

*Group picture before lunch

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

1:00	3:20	Sergei Kalinin (1:00-1:20) <ul style="list-style-type: none"> Integrating Autonomous Systems for Advanced Material Discovery: Bridging Experiments and Theory Through Optimized Rewards Mathew Cherukara (1:20-1:40) <ul style="list-style-type: none"> HPC+AI-enabled Materials Characterization and Experimental Automation Chris Stiles (1:40-2:00) <ul style="list-style-type: none"> Targeted AI-Driven Materials Discovery Break (2:00-2:20) Rama Vasudevan (2:20-2:40) <ul style="list-style-type: none"> Algorithms and opportunities for self-driving laboratories: model-based control, physics discovery, and co-navigating theory and experiments Maria Chan (2:40-3:00) <ul style="list-style-type: none"> Theory-informed AI/ML for materials characterization Yongqiang Cheng (3:00-3:20) <ul style="list-style-type: none"> Data-driven approaches to lattice dynamics and vibrational spectroscopy 	Invited Session II Chair: Howie Joress	
3:20	4:00	Sergei Kalinin, Hongliang Xin, Chris Stiles, Rama Vasudevan, Maria Chan, Vidushi Sharma, Timur Bazhirov	Panel Discussion Moderator: Brian DeCost	
4:00	5:30		Poster Session	

Agenda: Day 2

DATE: Day 2				
Start Time	End Time	Speaker(s)	Session Name/Information	AV/CS Notes:
8:45	11:45	Timur Bazhirov (8:45-9:05) <ul style="list-style-type: none"> Data Standards: the key enabler of AI-driven materials science at the nanoscale Vidushi Sharma (9:05-9:25) <ul style="list-style-type: none"> Chemical Foundation Models for Complex Materials Eddie Kim (9:25-9:45) <ul style="list-style-type: none"> A Practical Guide to Building with LLMs Anuroop Sriam (9:45-10:05) <ul style="list-style-type: none"> Beyond Experimental Structures: Advancing Materials Discovery with Generative AI Break (10:05-10:25)	Invited Session III Chair: Francesca Tavazza	Tian Xie is virtual
12:00	1:00		Lunch	
1:00	2:20	Michael Waters (1:00-1:20) <ul style="list-style-type: none"> Sampling Strategies for Robust MLIPs Guido von Rudorff (1:20-1:40)	Invited Session IV Chair: Kevin Garrity	

*Note, earlier start time for Day 2: 8:45am

		<ul style="list-style-type: none"> Unbiased Sampling of Chemical Space Olga Wodo (1:40-2:00)	
		<ul style="list-style-type: none"> Data-driven microstructure-property mapping: the importance of microstructure representation Keqiang Yang (2:00-2:20)	
2:30-4:30		<ul style="list-style-type: none"> Artificial Intelligence for Materials Geometric Representation Learning and High Tensor Order Property Predictions <ol style="list-style-type: none"> Peter Bajcsy (2:30-2:50) Austin McDannald (2:50-3:35) Brain DeCost/Daniel Wines/Kamal Choudhary (3:35-4:30) 	Hands On Session 1) NN Calculator Tutorial 2) Active Learning/Gaussian Processes 3) ALIGNN and ALIGNN-FF 4) Atom-GPT

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

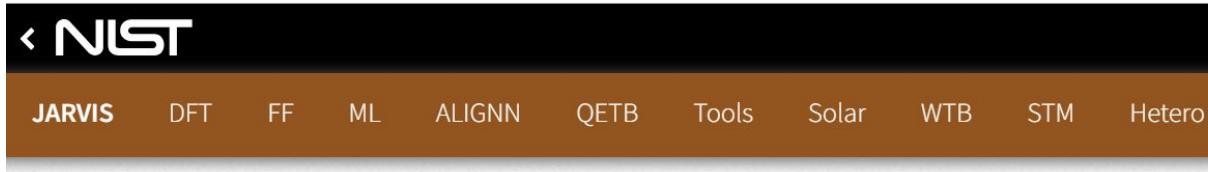
* For hands-on session: recommended to have

1) Gmail account, 2) JARVIS-account, 3) GitHub account

* Poster award for students/postdocs only, winner announcement on Day 2

JARVIS Overview

← → ⌂ jarvis.nist.gov



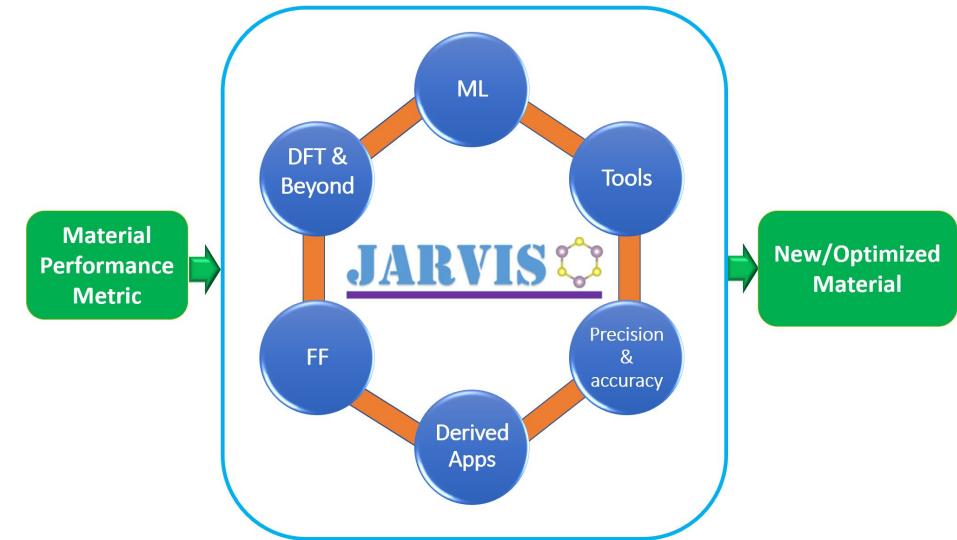
The JARVIS (Joint Automated Repository for Various Integrated Simulations) is a web-based platform designed to automate materials discovery and optimization using classical force-field learning, quantum computation calculations and experiments. Access to the system requires user credentials. User-registration is free, click on the [Login/Sign up button](#) in: [Nature Portfolio](#), [AIP](#) and [other publications](#). For upcoming events, c

Materials Genome Initiative 2011, \$400 million



<https://www.nist.gov>

<https://jarvis.nist.gov> (Estd. 2017)



US CHIPS Act 2022, \$52 billion

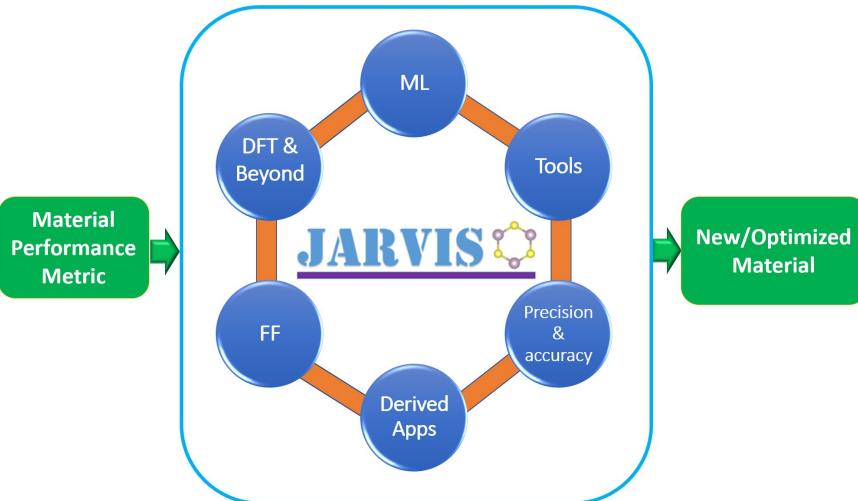


<https://nvlpubs.nist.gov/nistpubs/CHIPS/NIST.C>

JARVIS: Databases, Tools, Events, Outreach



<https://jarvis.nist.gov>



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

- Density functional theory (JARVIS-DFT)
- Force-field (JARVIS-FF)
- JARVIS-QETB (Density Functional Theory with Quantum Expresso for TB training)
- JARVIS-ALIGNN
- JARVIS-ML (Machine learning (CFID))
- JARVIS-WannierTB (Wannier tight-binding)
- Databases (including Materials Project, Materials API, and Materials Data API)
- Tools (including JARVIS-ML, JARVIS-FF, JARVIS-DFT, JARVIS-QETB, JARVIS-ALIGNN, and JARVIS-WannierTB)

Established: January 2017

Published: >45 articles, 3000+ citations

Users: >100000+ users worldwide

Materials: >80000, millions of properties

Events:

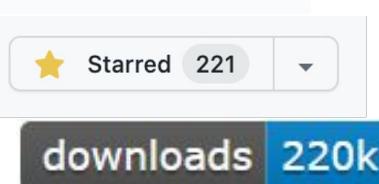
- Quantum Matters in Materials Science (QMMS)
- Artificial Intelligence for Materials Science (AIMS)
- JARVIS-School (**reach out if interested**)



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...”



Databases

Name	Database/WebApp	Description
1. JARVIS-DFT (DMFT,QMC)	https://jarvis.nist.gov/jarvisdft	Density functional theory DB for 80000+ materials, >million properties
2. JARVIS-FF	https://jarvis.nist.gov/jarvisff	Classical DB for ~2000 materials, >100 Classical FFs
3. JARVIS-CFID	https://jarvis.nist.gov/jarvisml	Classical force-field inspired (CFID) descriptors for conventional machine learning
4. ALIGNN, FF	https://github.com/usnistgov/alignn/	Atomistic Line Graph Neural Network for fast property prediction, unified FF for periodic table, structure optimization
5. AtomGPT	https://github.com/usnistgov/atomgpt	Atomistic Generative Pretrained transformer for forward and inverse materials design
6. InterMat	https://github.com/usnistgov/intermat	Interface Materials Design Toolkit with DFT and AI methods
7. ChemNLP	https://github.com/usnistgov/chemnlp	Natural language processing for materials chemistry for arXiv/pubchem data
8. DAC	https://jarvis.nist.gov/jdac	Direct air capture/CO ₂ capture with AI trained on GCMC data
9. Leaderboard	pages.nist.gov/jarvis_leaderboard	Large scale benchmark platform with >300 benchmarks, 9 million data points
10. AtomVision	https://github.com/usnistgov/atomvision	Computer vision models and dataset for materials science, STEM/STM
11. AtomQC	https://github.com/usnistgov/atomqc	Quantum computation library for molecules and solids
12. Tb3Py	https://github.com/usnistgov/tb3py	Three-body tight-binding model for the periodic table
13. Solar	https://jarvis.nist.gov/jsolar	Solar cell materials design with DFT, AI

jarvis.nist.gov/jarvisdft/

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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.

Search
Refresh

https://jarvis.nist.gov/jarvisdft/

how 100 entries

id	formula	Spg	SpgNum	crys	func	E_form	OPT_gap	MBJ_gap	hse_gap	Kv	Gv	poisson	spillage	slme	mag	type
JVASP-664	MoS2	P-6m2	187	hexagonal	OptB88vdW	-0.88454	1.658	-	-	-	-	-	0.003	-	0.0	2D
JVASP-730	MoS2	R-3m	166	trigonal	OptB88vdW	-0.60967	0.000	-	-	-	-	-	0.976	-	-0.0	2D
JVASP-100856	MoS3	P2_1/m	11	monoclinic	OptB88vdW	-0.34773	0.443	-	-	-	-	-	-	-	0.0	3D
JVASP-111117	MoS2	P-3m1	164	trigonal	OptB88vdW	-0.69305	0.000	0.0	-	-	-	-	-	-	0.0	3D
JVASP-127507	MoS	Pm-3m	221	cubic	OptB88vdW	-0.18293	0.000	-	-	-	-	-	-	-	0.0	3D
JVASP-132473	MoS3I	P1	1	triclinic	OptB88vdW	0.06061	0.651	-	-	-	-	-	-	-	3.993	3D
JVASP-144515	Mo3S4	P-1	2	triclinic	OptB88vdW	-0.73826	0.000	-	-	-	-	-	-	-	0.0	3D
JVASP-228	MoS2	R-3m	166	trigonal	OptB88vdW	-0.69909	0.000	0.0	-	51.32	45.47	0.19	0.852	-	0.0	3D
JVASP-28379	MoS2	P6_3/mmc	194	hexagonal	OptB88vdW	-0.95754	0.958	1.364	-	71.48	44.27	0.26	-	33.92	-	3D
JVASP-28413	MoS2	P-3m1	164	trigonal	OptB88vdW	-0.92268	1.207	1.471	-	-	-	-	-	32.7	0.0	3D
JVASP-28733	MoS2	P6_3/mmc	194	hexagonal	OptB88vdW	-0.96160	0.921	-	-	70.82	47.69	0.23	0.013	-	0.0	3D
JVASP-34138	MoS2	P6_3/mmc	194	hexagonal	OptB88vdW	-0.96135	0.920	1.356	-	-	-	-	-	33.93	0.0	3D

[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): 0.866	Volume (Å ³): 308.988	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: 0.069	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. RD phonon (cm ⁻¹):	Cut-off (eV): 850	K-point length (Å): 25

[Show POSCAR](#) [Show POSCARconv](#) [Show XYZ format](#) [Show CIF format](#)

Visualizing Atomic structure

Atomic Structure Analysis

The following shows the radial, angle and dihedral distribution function plots.

Distance (Å)

Distance (Å)

Angle upto first neighbor

Angle upto first neighbor

Dih. angle upto first neighbor

Dih. angle upto first neighbor

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)

High-throughput Identification and Characterization of Two-dimensional Materials using Density functional theory

Kamal Choudhary , Irina Kalish, Ryan Beams & Francesca Tavazza

Scientific Reports 7, Article number: 5179 (2017) | [Cite this article](#)

Computational screening of high-performance optoelectronic materials using OptB88vdW and TB-mBJ formalisms

Kamal Choudhary , Qin Zhang, Andrew C.E. Reid, Sugata Chowdhury, Nhan Van Nguyen, Zachary Trau

Marcus W. Newrock, Faical Yannick Congo & Francesca Tavazza

Accelerated Discovery of Efficient Solar Cell Materials Using Quantum and Machine-Learning Methods

Kamal Choudhary*, Marnik Bercx, Jie Jiang, Ruth Pachter, Dirk Lamoen, and Francesca Tavazza

 [Cite this: Chem. Mater.](#) 2019, 31, 15, 5900–5908

Publication Date: July 17, 2019 ✓

<https://doi.org/10.1021/acs.chemmater.9b02166>

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RIS

High-throughput density functional perturbation theory and machine learning predictions of infrared, piezoelectric, and dielectric responses

Kamal Choudhary , Kevin F. Garrity, Vinit Sharma, Adam J. Biacchi, Angela R. Hight Walker & Francesca

Tavazza

npg Computational Materials 6, Article number: 64 (2020) | [Cite this article](#)

Data-driven discovery of 3D and 2D thermoelectric materials

Kamal Choudhary^{2,1} , Kevin F Garrity¹ and Francesca Tavazza¹

Published 27 August 2020 • © 2020 IOP Publishing Ltd

Journal of Physics: Condensed Matter, Volume 32, Number 47

Citation Kamal Choudhary et al 2020 *J. Phys.: Condens. Matter* 32 475501

High-throughput Discovery of Topologically Non-trivial Materials using Spin-orbit Spillage

Kamal Choudhary , Kevin F. Garrity & Francesca Tavazza

Scientific Reports 9, Article number: 8534 (2019) | [Cite this article](#)

Designing high- T_c superconductors with BCS-inspired screening, density functional theory, and deep-learning

Kamal Choudhary & Kevin Garrity

npg Computational Materials 8, Article number: 244 (2022) | [Cite this article](#)

High-Throughput DFT-Based Discovery of Next Generation Two-Dimensional (2D) Superconductors

Daniel Wines*, Kamal Choudhary, Adam J. Biacchi, Kevin F. Garrity, and Francesca Tavazza

 [Cite this: Nano Lett.](#) 2023, 23, 3, 969–978

Publication Date: January 30, 2023 ✓

<https://doi.org/10.1021/acs.nanolett.2c04420>

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Predicting anomalous quantum confinement effect in van der Waals materials

Kamal Choudhary and Francesca Tavazza

Phys. Rev. Materials 5, 054602 – Published 7 May 2021

Can a deep-learning model make fast predictions of vacancy formation in diverse materials?

Kamal Choudhary ; Bobby G. Sumpter 

 Check for updates

+ Author & Article Information

AIP Advances 13, 095109 (2023)



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)}

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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



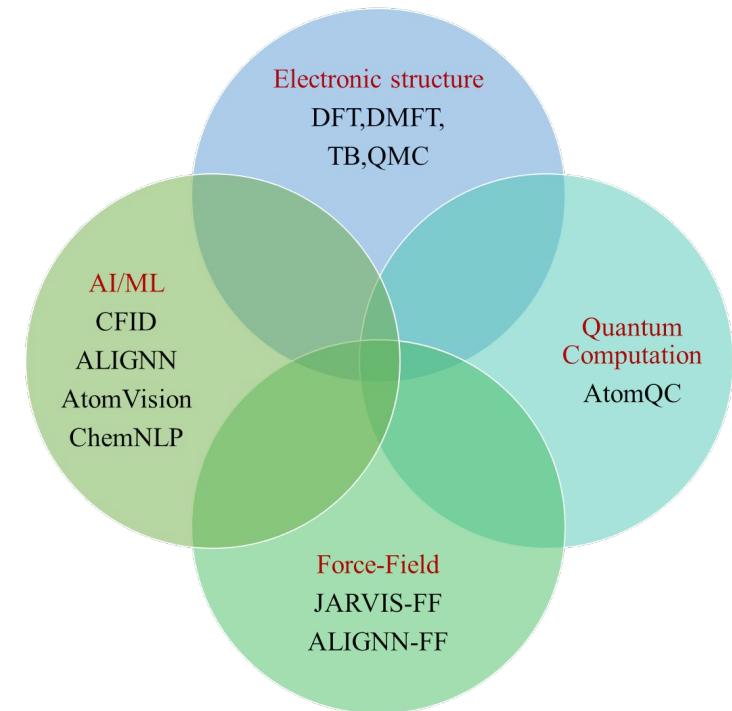
Cite this: DOI: [10.1039/d2dd00096b](https://doi.org/10.1039/d2dd00096b)



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

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

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



Latest Projects

ALIGNN

This app predicts properties of an input material given in POSCAR format using JARVIS-ALIGNNN

Mo1 Se2
1.0
1.681759 -2.878250 0.000000
1.681759 2.878250 0.000000
0.000000 0.000000 35.451423
Mo Se
1 2
direct
0.666667 0.333333 0.326886 Mo
0.333333 0.666667 0.370808 Se
0.333333 0.666667 0.279691 Se

Model	MAE	Team	Date submitted	Notes
JARVIS-ALIGNNN	0.0271	JARVIS	05/09/2023	CSV, JSON, vac, chg, info
JARVIS-ALIGNNN	0.0291	JARVIS	05/09/2023	CSV, JSON, vac, chg, info
potfit	0.0293	DFT@TAMU	05/13/2023	CSV, JSON, vac, chg, info
mediumer_298	0.0822	DFT@TAMU	05/13/2023	CSV, JSON, vac, chg, info
algnn.model	0.0831	ALGNN	05/13/2023	CSV, JSON, vac, chg, info
algnn.jarvis	0.0345	JARVIS	05/13/2023	CSV, JSON, vac, chg, info
algnn.jarvis10	0.0423	JARVIS	05/09/2023	CSV, JSON, vac, chg, info
algnn.dimera10	0.0528	JARVIS	05/09/2023	CSV, JSON, vac, chg, info
algnn.dimera	0.0861	JARVIS	05/13/2023	CSV, JSON, vac, chg, info
algnn.model	0.0625	COON	05/13/2023	CSV, JSON, vac, chg, info

- <https://github.com/usnistgov/alignn>
- <https://jarvis.nist.gov/jalignn/>
- Atomistic Line Graph Neural Network (bond-angles)
- Pretrained ML model 70+ materials properties
- Unified GNN force-field for 89 elements
- NPJ Comput. Mater. (2021)
- Digital Discovery (2023)

JARVIS-Leaderboard

(a) Homepage snapshot

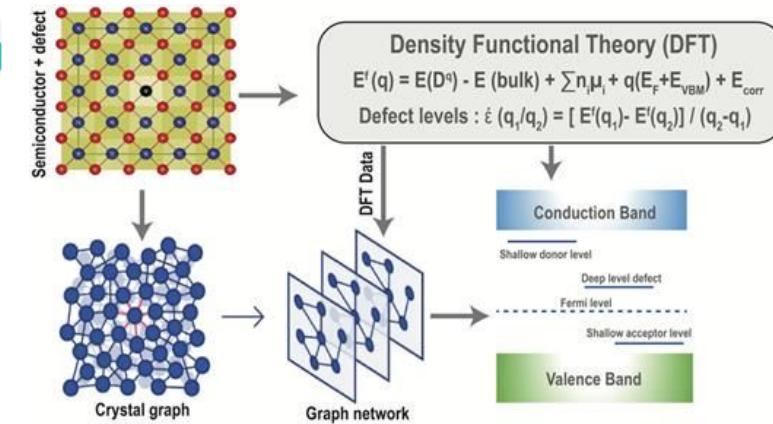
(b) AI formation energy example plot

(c) AI formation energy example table

Model name	Dataset	MAE	Team name	Dataset size	Date submitted	Notes
algnn.dimera	dft_3d	0.0271	JARVIS	55713	05/09/2023	CSV, JSON, vac, chg, info
algnn.dimera	dft_3d	0.0291	JARVIS	55713	05/09/2023	CSV, JSON, vac, chg, info
potfit	dft_3d	0.0293	DFT@TAMU	55713	05/13/2023	CSV, JSON, vac, chg, info
mediumer_298	dft_3d	0.0822	DFT@TAMU	55713	05/13/2023	CSV, JSON, vac, chg, info
algnn.model	dft_3d	0.0831	ALGNN	55713	05/13/2023	CSV, JSON, vac, chg, info
algnn.jarvis	dft_3d	0.0345	JARVIS	55713	05/13/2023	CSV, JSON, vac, chg, info
algnn.jarvis10	dft_3d	0.0423	JARVIS	55713	05/09/2023	CSV, JSON, vac, chg, info
algnn.dimera10	dft_3d	0.0528	JARVIS	55713	05/09/2023	CSV, JSON, vac, chg, info
algnn.dimera	dft_3d	0.0861	JARVIS	55713	05/13/2023	CSV, JSON, vac, chg, info
algnn.model	dft_3d	0.0625	COON	55713	05/13/2023	CSV, JSON, vac, chg, info

- https://pages.nist.gov/jarvis_leaderboard/
- Unified benchmarking platform for transparent & reproducible benchmarking
- AI, FF, ES, QC, Exp methods
- 9 million+ datapoints
- 300+ benchmarks
- 1700 contributions
- 20+ contributors
- NPJ Comput. Mater. (2024)

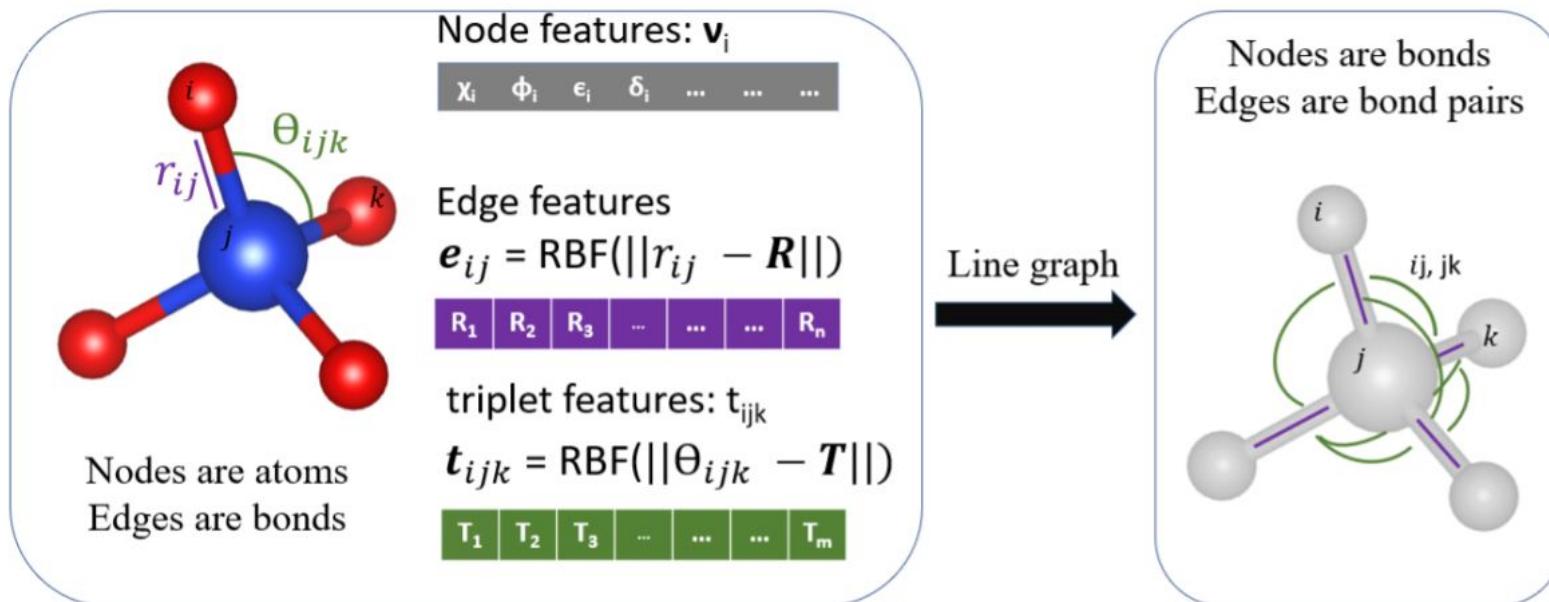
DefectMat



- ALIGNN+DFT for accelerated defect design,
- Benchmarked vacancy formation predictions,
- Neutral and charged defects,
- AIP Advances 2023,
- APL Machine Learning 2024

Atomistic Graph & Line Graph

Explicitly represent pairwise and triplet (bond angle) interactions using line graph
Possible to extend for n-body, e.g. line graph of line graph



- Graph level prediction, e.g. energy
- Node level predictions, e.g. charges
- Node level derivatives, e.g. forces
- Edge level predictions, e.g. LJ params

npj | computational materials

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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



Digital Discovery

PAPER



View Article Online
View Journal

Check for updates
Cite this: DOI: 10.1039/d2dd00096b

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

Kamal Choudhary, ^{a,b} Brian DeCost, ^{b,c} Lily Major, ^{b,d,e} Keith Butler, ^{b,e} Jeyan Thiagaralingam ^{b,e} and Francesca Tavazza ^{b,c}

High Pressure Hydride Superconductors

NIST

PAPER • OPEN ACCESS

Data-driven design of high pressure hydride superconductors using DFT and deep learning

Daniel Wines^{2,1}  and Kamal Choudhary¹ 

Published 31 May 2024 • © 2024 The Author(s). Published by IOP Publishing Ltd on behalf of the Songshan Lake

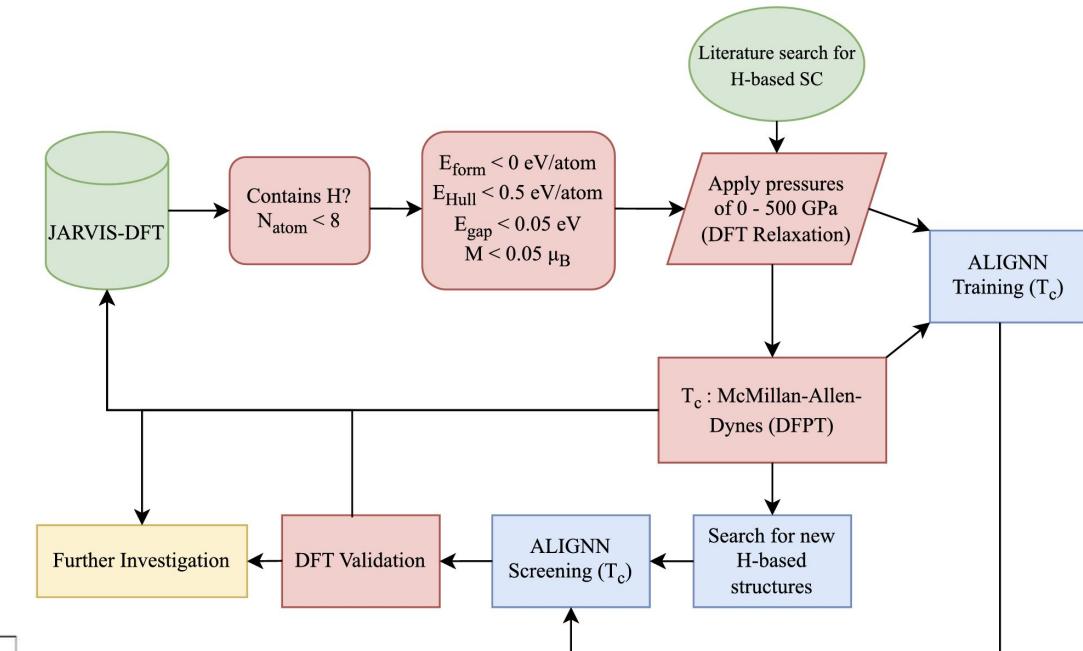
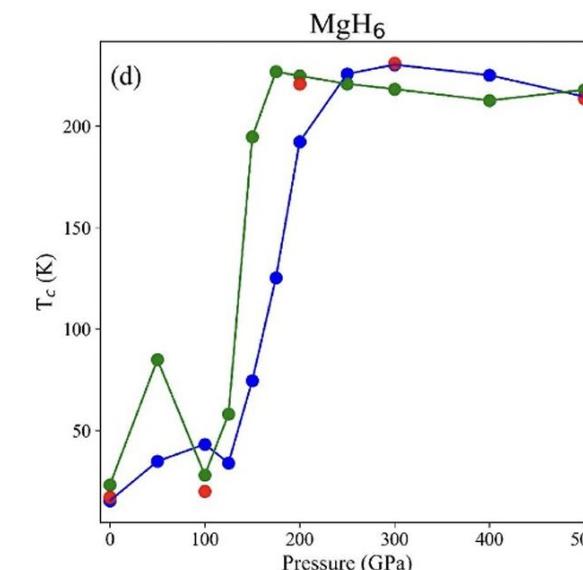
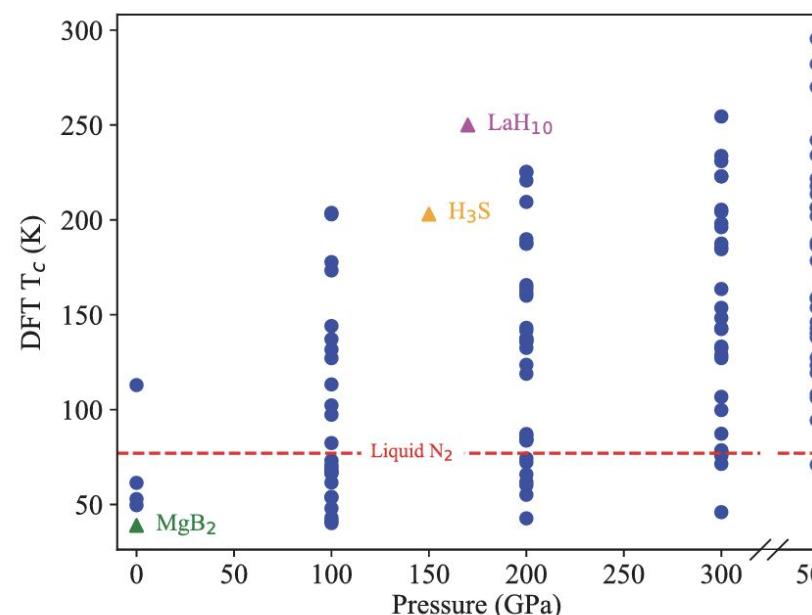
Materials Laboratory

[Materials Futures, Volume 3, Number 2](#)

[Focus Issue on Artificial Intelligence for Materials Science](#)

Citation Daniel Wines and Kamal Choudhary 2024 *Mater. Futures* 3 025602

DOI 10.1088/2752-5724/ad4a94



- Performed **DFT** calculations for **~950** high pressure hydride superconductors (T_c)
- Trained **ALIGNN** model to predict T_c
- Applied **ALIGNN-FF** and **ALIGNN-SC** model to predict T_c under pressure
- Models extrapolate well to intermediate pressure values (not part of training)
- Can provide qualitative landscape of hydrides under pressure

Latest Projects

ALIGNN

This app predicts properties of an input material given in POSCAR format using JARVIS-ALIGNNN

Mo1 Se2	1.0
1.681759 -2.878250 0.000000	
1.681759 2.878250 0.000000	
0.000000 0.000000 35.451423	
Mo Se	1 2
direct	
0.666667 0.333333 0.326886 Mo	
0.333333 0.666667 0.370808 Se	
0.333333 0.666667 0.279691 Se	

- <https://github.com/usnistgov/alignn>
- <https://jarvis.nist.gov/jalignn/>
- Atomistic Line Graph Neural Network (bond-angles)
- Pretrained ML model 70+ materials properties
- Unified GNN force-field for 89 elements
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- Digital Discovery (2023)

JARVIS-Leaderboard

(a) Homepage snapshot

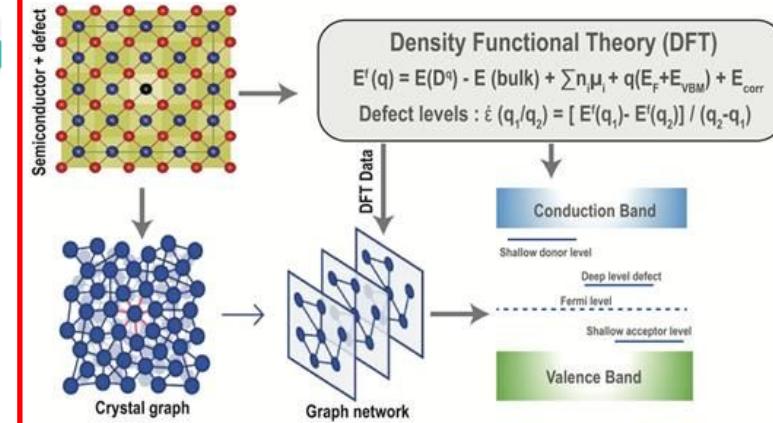
(b) AI formation energy example plot

(c) AI formation energy example table

Model name	Dataset	MAE	Team name	Dataset size	Date submitted	Notes
alignn_2023	dft_3d	0.0271	alignn	55713	0549-2023	CSV, JSON, nancv, info
alignn_2023	dft_3d	0.0291	alignn	55713	0549-2023	CSV, JSON, nancv, info
potfit	dft_3d	0.0293	DFT@TAMU	55713	06-02-2023	CSV, JSON, nancv, info
mediumcar_2023	dft_3d	0.0322	DFT@TAMU	90713	0641-2023	CSV, JSON, nancv, info
alignn_2023	dft_3d	0.0331	alignn	55713	01-14-2023	CSV, JSON, nancv, info
alignn_2023	dft_3d	0.0345	alignn	55713	09-29-2023	CSV, JSON, nancv, info
alignn_2023	dft_3d	0.0423	alignn	55713	05-06-2023	CSV, JSON, nancv, info
alignn_2023	dft_3d	0.0528	alignn	55713	05-06-2023	CSV, JSON, nancv, info
alignn_2023	dft_3d	0.0681	alignn	55713	09-26-2023	CSV, JSON, nancv, info
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- Benchmarked vacancy formation predictions,
- Neutral and charged defects,
- AIP Advances 2023,
- APL Machine Learning 2024

Reproducibility & Benchmarking



Challenges in materials science community:

- Reproducibility
- Transparency
- Validation
- Fidelity
- Data vs. metadata
- What is the ground truth/reference?

Synergy of computational and experimental databases

1,500 scientists lift the lid on reproducibility

[Monya Baker](#)

[Nature](#) 533, 452–454 (2016) | [Cite this article](#)

171k Accesses | 1952 Citations | 5176 Altmetric | [Metrics](#)

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

The screenshot shows the homepage of the JARVIS-Leaderboard. At the top, there's a navigation bar with the NIST logo, a menu icon, the page title "JARVIS-Leaderboard", a search bar, and a status bar indicating "jarvis_leaderboard v2024.1.26 ☆44 28". Below the header, a main title reads "Explore State-of-the-Art Materials Design Methods". The page is divided into four main sections, each containing a card with a title, contribution count, and a "See All Benchmarks" link. The sections are: Artificial intelligence (AI) with 607 contributions, Electronic Struct. (ES) with 786 contributions, Force-field (FF)/potentials with 282 contributions, and Quantum Comput. (QC) with 6 contributions. Below these are two more sections: Experiments (EXP) with 25 contributions and Example Notebooks with 16 notebooks, both with "See All Benchmarks" links. The final section is Methodologies with 385 available methods, a "Learn more" button, and a "Contribution Guide" link with 21 contributors.

Methodology	Contributions	Action
Artificial intelligence (AI)	607	See All Benchmarks
Electronic Struct. (ES)	786	See All Benchmarks
Force-field (FF)/potentials	282	See All Benchmarks
Quantum Comput. (QC)	6	See All Benchmarks
Experiments (EXP)	25	See All Benchmarks
Example Notebooks	16	See All Notebooks
Methodologies	385	Learn more
Contribution Guide	21	Learn more

Goals

1. Flexibility to add new benchmarks
2. Experimental round-robin studies
3. Multi-modality: benchmarks beyond AI/ML/atomistic property
4. Easy to use/ get started
5. worked out examples (Jupyter/Colab notebooks)

Categories of benchmarks

JARVIS-Leaderboard: a large scale benchmark of materials design methods

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, Arun Mannodi-Kanakkithodi, Elif Ertekin, Avanish Mishra, Nithin Mathew, Mitchell Wood, Andrew Dale Rohskopf, Jason Hattrick-Simpers, Shih-Han Wang, Luke E. K. Achenie, Hongliang Xin, Maureen Williams, Adam J. Baciotti & Francesca Tavazza  — Show fewer authors

npj Computational Materials 10, Article number: 93 (2024) | [Cite this article](#)

Category	General name	Method Specification
ES	DFT ⁶⁴	VASP ^{52,53} (PBE ⁵⁴ , LDA ⁶⁴ , OptB88vdW ⁶⁵ , Opt86BvdW ⁶⁶ , TBmBJ ^{67,68} , SCAN ⁶⁹ , r2SCAN ⁷⁰ , HSE06 ⁷¹) QE ⁷² (PBE ⁵⁴ , PBEsol ⁷³) ABINIT ^{74–76} (PBE ⁵⁴) GPAW ⁷⁷ (PBE ⁵⁴ , LDA ⁶⁴ , GLLB-sc ⁷⁸)
	QMC ⁶¹	QMCPACK ⁷⁹ (DMC ⁶¹)
	GW ⁶³	VASP ^{52,53} (G_0W_0 ⁶³ , GW ₀ ⁶³)
	TB ⁵⁷	ThreeBodyTB.jl ⁵⁹ (Wannier90 ⁸⁰)
AI	Descriptor	CFID ⁸¹ , MagPie ⁸² , MatMiner ^{55,83} , crystal feature model ⁸⁴ , ElemNet ^{85–87} , IRNet ^{88–90} , BRNet ^{91,92} , SNAP ⁹³
	Graph-based	ALIGNN ⁹⁴ , CGCNN ⁹⁵ , SchNet ⁹⁶ , AtomVision ⁹⁷ , ChemNLP ⁹⁸ , DimeNet ^{99,100} , CHGNet ¹⁰¹ , M3GNET ¹⁰² , kgcnn_coGN ¹⁰³ , Potnet ¹⁰⁴ , Matformer ¹⁰⁵
	Transformers	OPT ¹⁰⁶ , GPT ¹⁵ , T5 ¹⁰⁷
FF	LJ ¹⁰⁸	LAMMPS ¹⁰⁹ (2D-Liquid)
	EAM ¹¹⁰	LAMMPS ¹⁰⁹ (FCC-Al)
	REBO ¹¹¹	LAMMPS ¹⁰⁹ (Diamond-Si)
	AMBER99sb-ildn ¹¹²	GROMACS ¹¹³ (Alanine dipeptide)
QC	CHARMM36m ¹¹⁴	GROMACS ¹¹³ (α -aminoisobutyric acid)
	Algorithms	Qiskit ¹¹⁵ (VQE ¹¹⁶ , VQD ¹¹⁷) PennyLane ^{118,119} (VQE ¹¹⁶ , VQD ¹¹⁷)
	Circuits	Qiskit ¹¹⁵ (PauliTwo Design ¹¹⁵ , SU(2) ¹¹⁵)
EXP	Diffraction	XRD (Bruker D8)
	Manometry	CO ₂ adsorption FACT lab ¹²⁰
	Vibroscopy	Kevlar FAVIMAT ¹²¹
	Magnetometry	Susceptibility (PPMS) ¹²¹

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

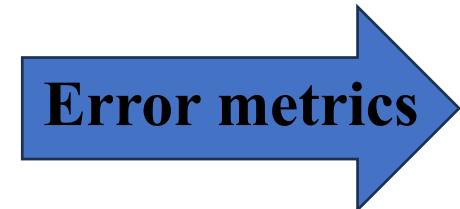
Types of Data:

- **Atomic structure** (Molecule, Crystal)
- **Material Property** (Bandgap, bulk modulus)
- **Images** (Microscopy: SEM, TEM, STM)
- **Spectra** (Diffraction: X-ray, Neutron, PL)
- **Text** (Research articles, notebooks, blogs)
- **Eigensolver** (Quantum Computation algorithms)



Contributions

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



Benchmarks (reference point)

- 1) Experiment(s)
- 2) Test dataset
- 3) Electronic Structure
- 4) Analytical results
- 5) Other Experiments

*Benchmarks must be well-defined with an associated DOI

Coming soon: ReproHack (Reproducibility Hackathon), Sept. 16, 2024
<https://forms.gle/pn75ZjwBJvDxaKTh9>

Latest Projects

ALIGNN

This app predicts properties of an input material given in POSCAR format using JARVIS-ALIGNNN

Mo1 Se2
1.0
1.681759 -2.878250 0.000000
1.681759 2.878250 0.000000
0.000000 0.000000 35.451423
Mo Se
1 2
direct
0.666667 0.333333 0.326886 Mo
0.333333 0.666667 0.374080 Se
0.333333 0.666667 0.279691 Se

Submit

Model	MAE	Team	Date submitted	Notes
JARVIS-ALIGNNN	0.0271	JARVIS	05/09/2023	CSV, JSON, XML, Info
JARVIS-ALIGNNN	0.0291	JARVIS	05/09/2023	CSV, JSON, XML, Info
potfit	0.0293	DFT@TAMU	05/13/2023	CSV, JSON, XML, Info
mediumer_298	0.0822	DFT@TAMU	05/13/2023	CSV, JSON, XML, Info
algnn.model	0.0831	ALGN	05/13/2023	CSV, JSON, XML, Info
algnn.jarvis	0.0345	JARVIS	05/13/2023	CSV, JSON, XML, Info
algnn.jarvis	0.0423	JARVIS	05/09/2023	CSV, JSON, XML, Info
algnn.dimera10	0.0528	JARVIS	05/06/2023	CSV, JSON, XML, Info
algnn.dimera10	0.1061	JARVIS	05/13/2023	CSV, JSON, XML, Info
algnn.dimera10	0.0625	CDONN	05/13/2023	CSV, JSON, XML, Info

JARVIS-Leaderboard

(a) Homepage snapshot

Explore State-of-the-Art Materials Design Methods

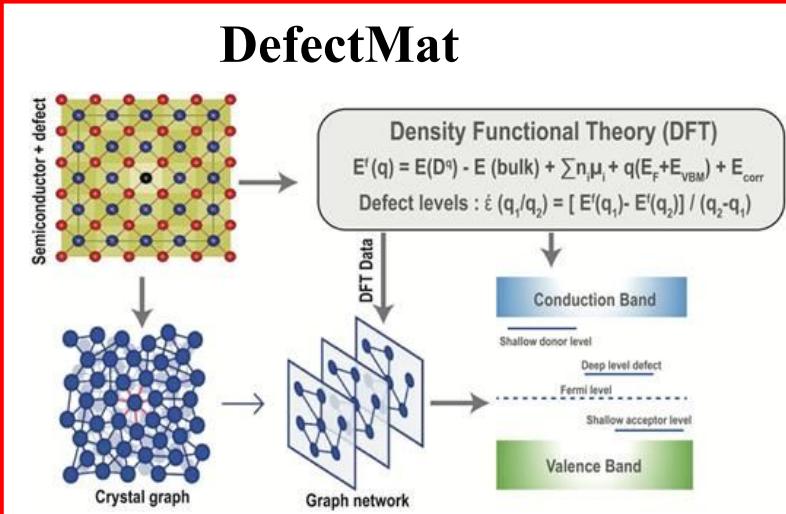
Model benchmarks

Model name	Dataset	MAE	Team name	Dataset size	Date submitted	Notes
algnn.dimera10	dft_3d	0.0271	JARVIS	55713	05/09/2023	CSV, JSON, XML, Info
algnn.dimera10	dft_3d	0.0291	JARVIS	55713	05/09/2023	CSV, JSON, XML, Info
potfit	dft_3d	0.0293	DFT@TAMU	55713	05/13/2023	CSV, JSON, XML, Info
mediumer_298	dft_3d	0.0822	DFT@TAMU	55713	05/13/2023	CSV, JSON, XML, Info
algnn.model	dft_3d	0.0831	ALGN	55713	05/13/2023	CSV, JSON, XML, Info
algnn.jarvis	dft_3d	0.0345	JARVIS	55713	05/13/2023	CSV, JSON, XML, Info
algnn.jarvis	dft_3d	0.0423	JARVIS	55713	05/09/2023	CSV, JSON, XML, Info
algnn.dimera10	dft_3d	0.0528	JARVIS	55713	05/06/2023	CSV, JSON, XML, Info
algnn.dimera10	dft_3d	0.1061	JARVIS	55713	05/13/2023	CSV, JSON, XML, Info
algnn.dimera10	dft_3d	0.0625	CDONN	55713	05/13/2023	CSV, JSON, XML, Info

(b) AI formation energy example plot

(c) AI formation energy example table

DefectMat

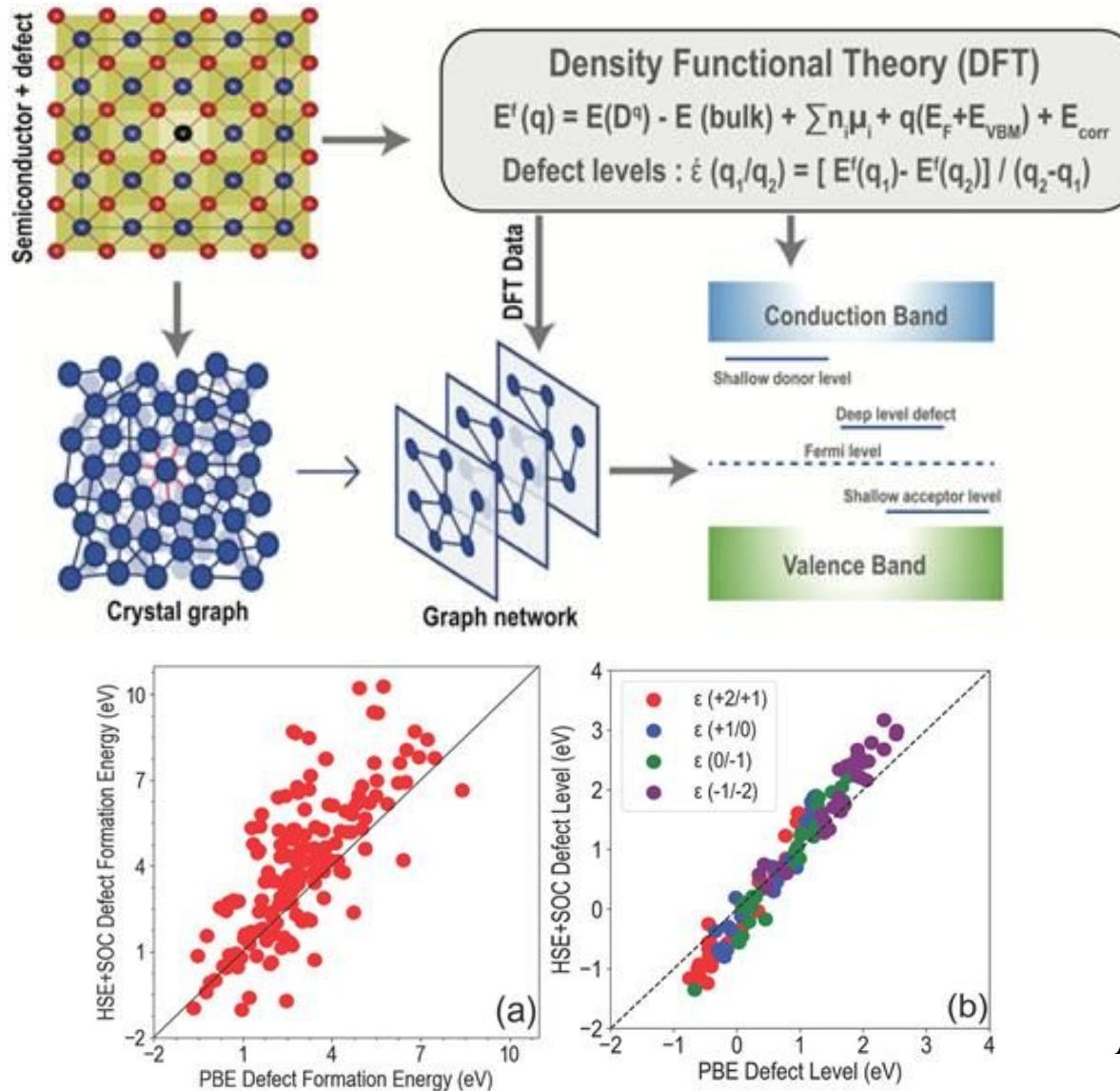


- <https://github.com/usnistgov/alignn>
- <https://jarvis.nist.gov/jalignn/>
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- Pretrained ML model 70+ materials properties
- Unified GNN force-field for 89 elements
- NPJ Comput. Mater. (2021)
- Digital Discovery (2023)

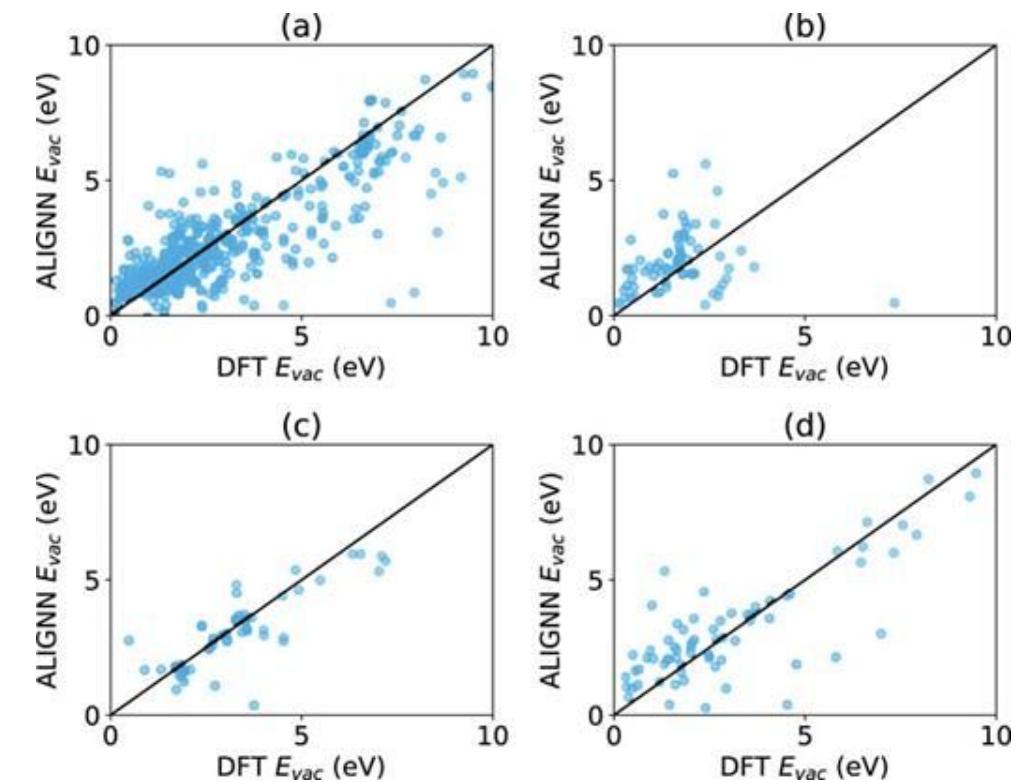
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- ALIGNN+DFT for accelerated defect design,
- Benchmarked vacancy formation predictions,
- Neutral and charged defects,
- AIP Advances 2023,
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DefectMat: Defect Materials Design



- ALIGNN+DFT for accelerated defect design
- Benchmarked vacancy formation predictions
- Neutral and charged defects

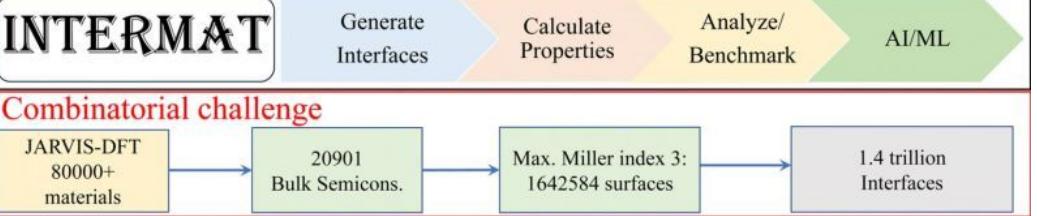


Latest Projects

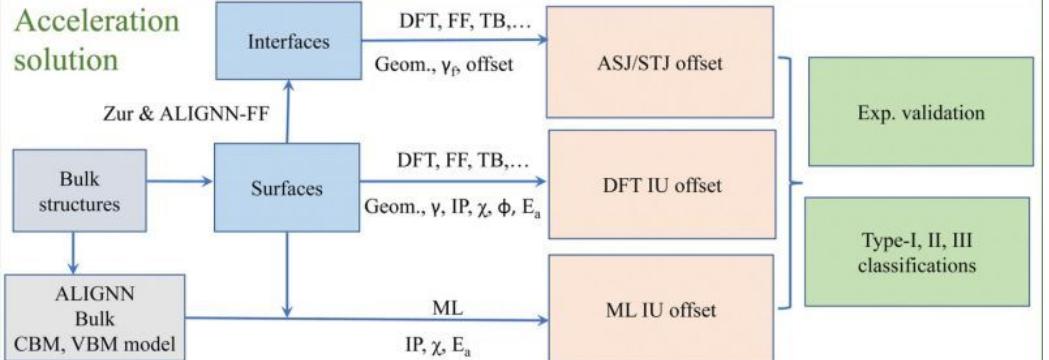
InterMat

INTERMAT

Combinatorial challenge

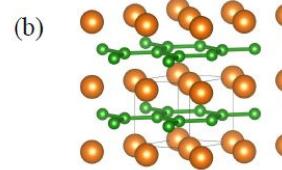
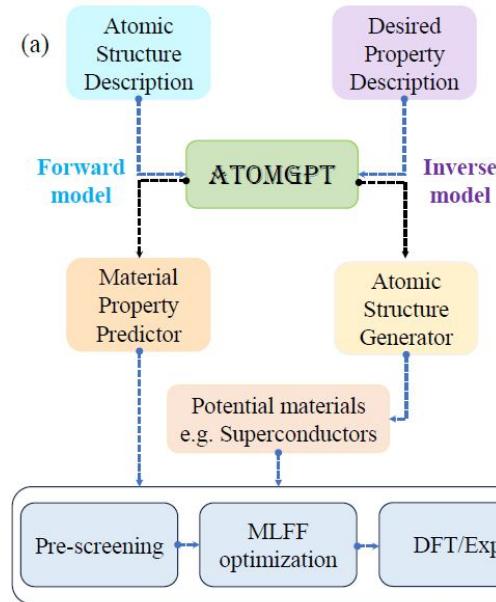


Acceleration solution



- <https://github.com/usnistgov/intermat>
- Interface materials design toolkit
- 1.4 trillion candidate semiconductor interfaces (largest ever) analyzed with deeplearning
- Independent unit (IU), Alternate slab junction (ASJ) and Exp. Validation
- Digital Discovery (2024)

AtomGPT

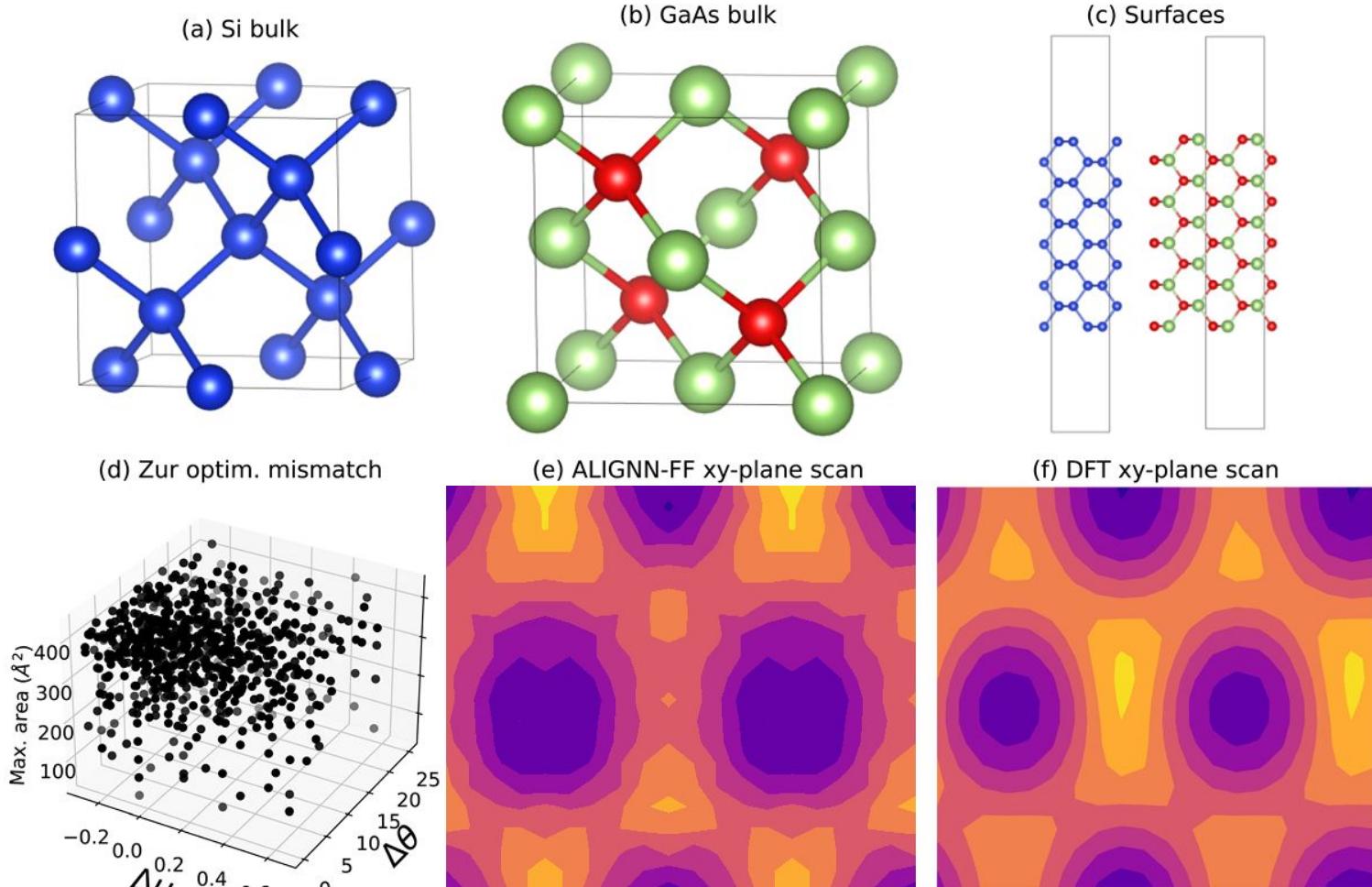


(c) **ChemNLP describer input:**
MgB₂ is crystallizes in the hexagonal P6/mmm space group. There is one shorter (2.5 Å) and one longer (3.96 Å) B-Mg bond lengths. Mg is bonded in edge-sharing MgB₁₂ Cuboctahedral...
Output: 32.685

(d) **Alpaca input:**
Instruction: Below is a description of a superconductor material..
Input: The chemical formula is MgB₂. The T_c_supercon is 32.685. Generate atomic structure description with lattice lengths, angles, coordinates and atom types..
Output: 3.07 3.07 3.51\n90 90 120\nMg 0.000 0.000 0.000\nB 0.667 0.333 0.500\nB 0.333 0.667 0.500}

- J. Phys. Chem. Lett., 2024
- Prompt based forward & inverse materials design
- Computational discovery of a novel superconductor candidate material using:
 - ✓ Large language models (LLM) (Inverse),
 - ✓ Machine learning (ML) surrogate models (Forward),
 - ✓ Machine-learning force-field (MLFF) (Geom. Optm.),
 - ✓ Density functional theory (DFT) (T_C predictions).

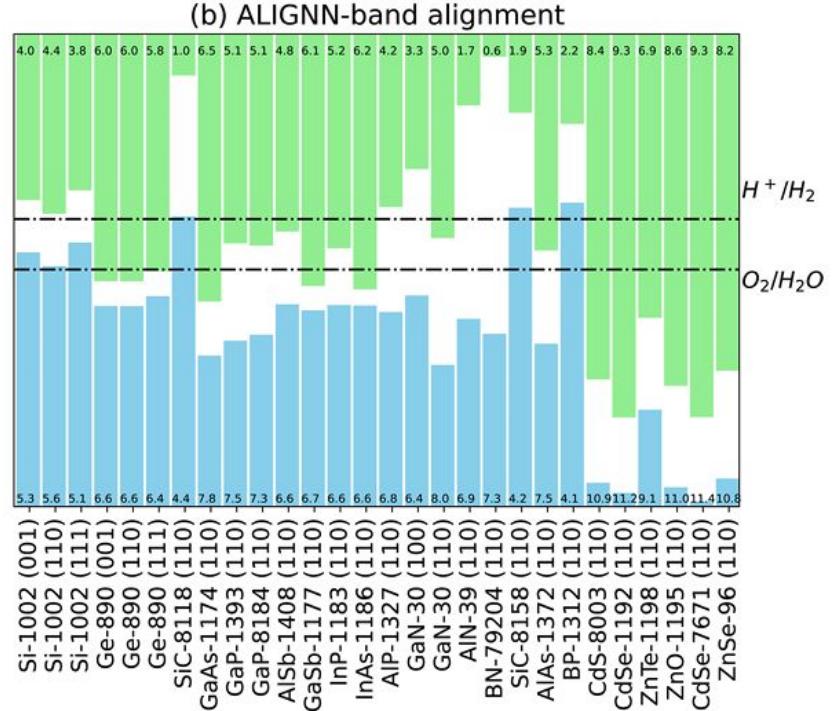
InterMat: Interface Materials Design (Semicons)



InterMat: accelerating band offset prediction in semiconductor interfaces with DFT and deep learning^t

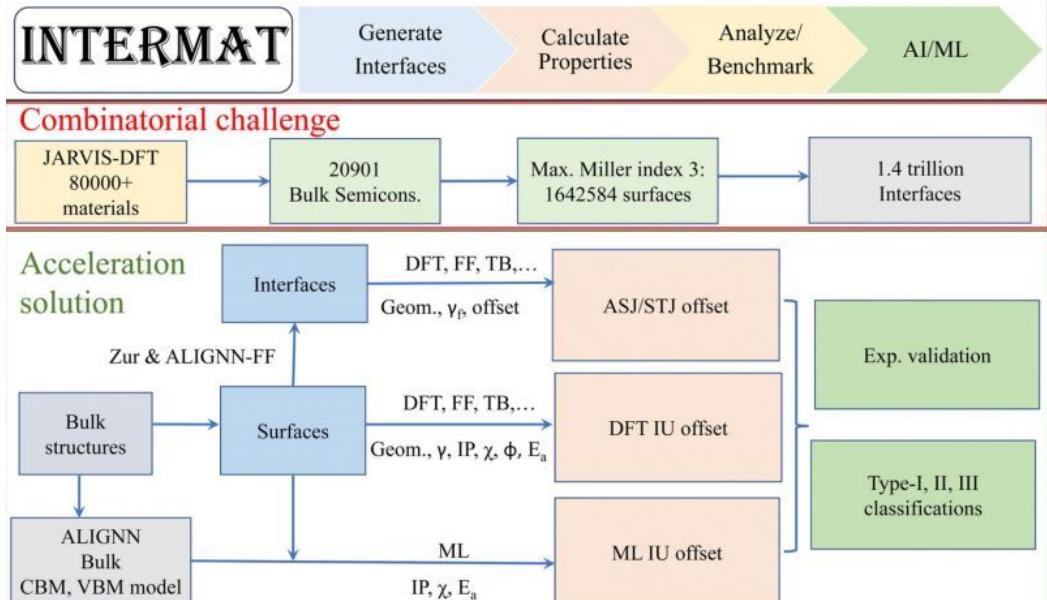
DOI: [10.1039/D4DD00031E](https://doi.org/10.1039/D4DD00031E) [Digital Discovery](#), 202

- ALIGNN+DFT for accelerated interface design
- Benchmarked band-offset predictions
- General workflow for materials design



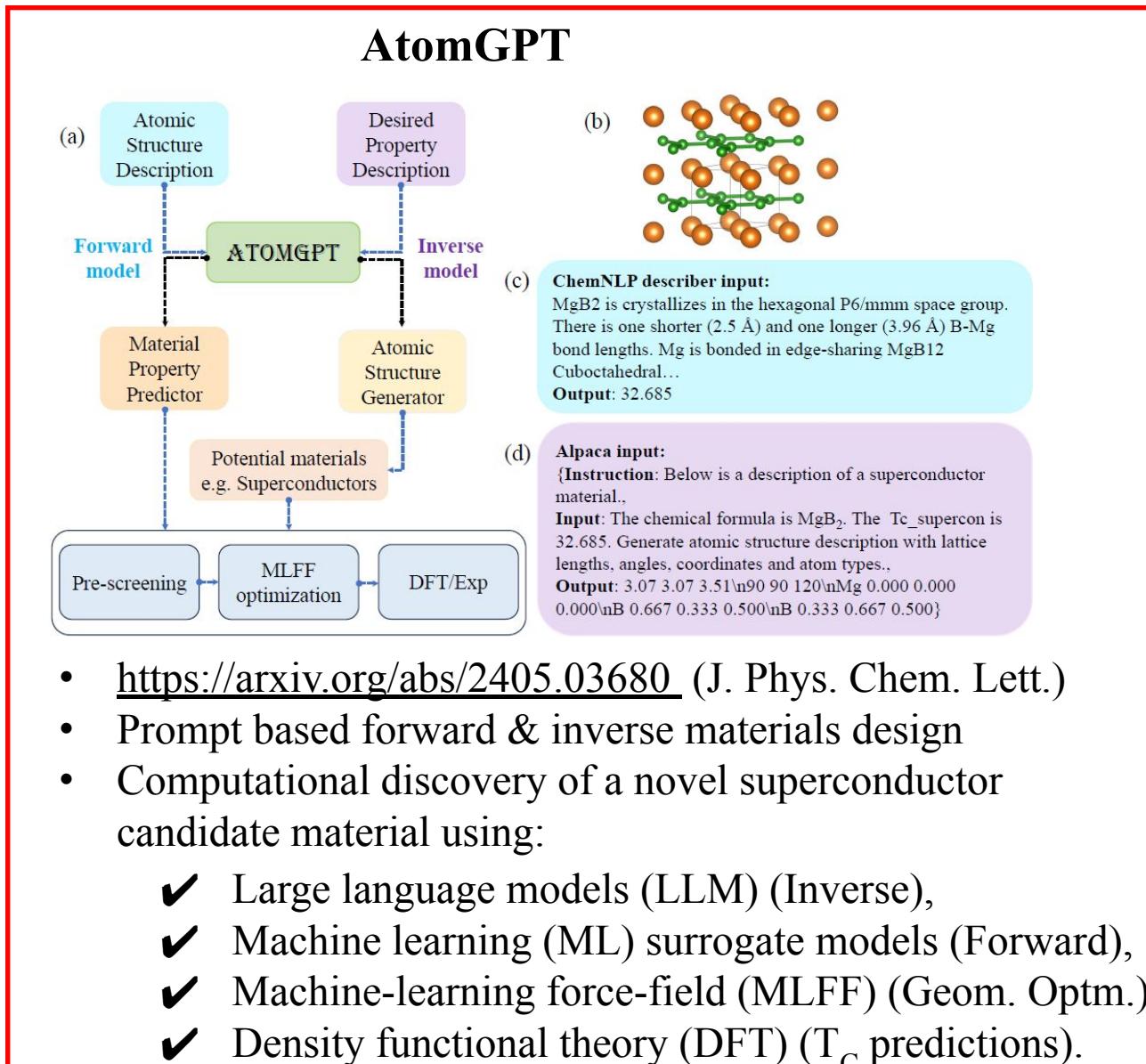
Latest Projects

InterMat



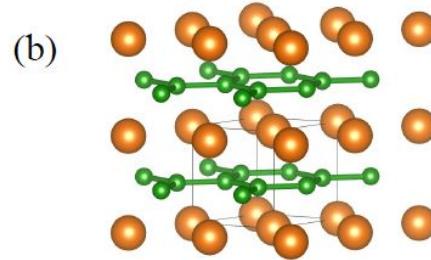
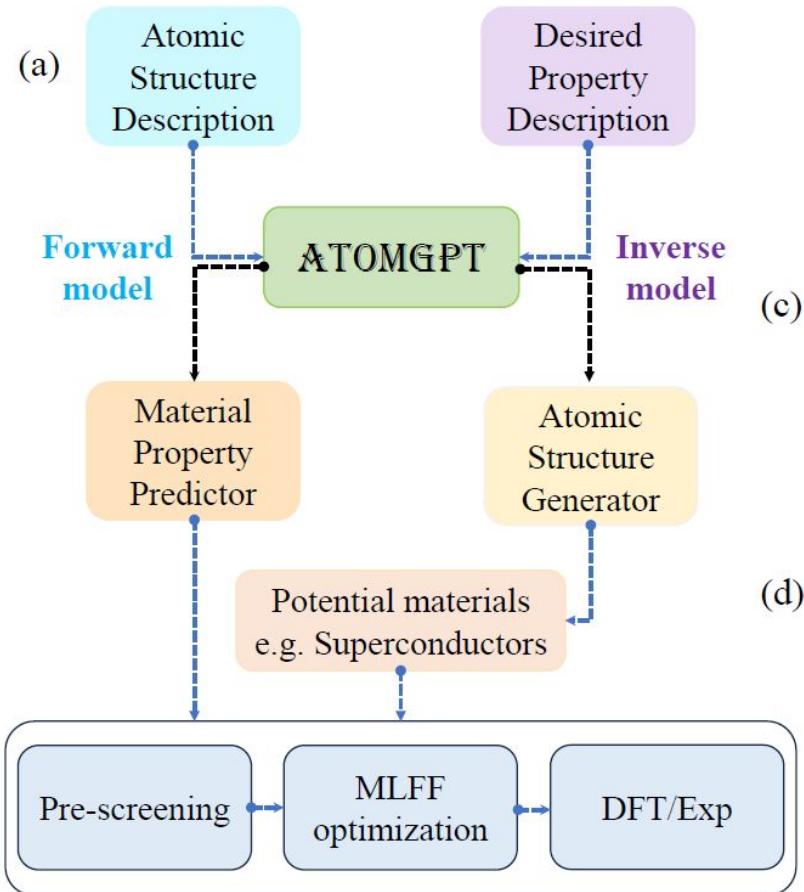
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AtomGPT

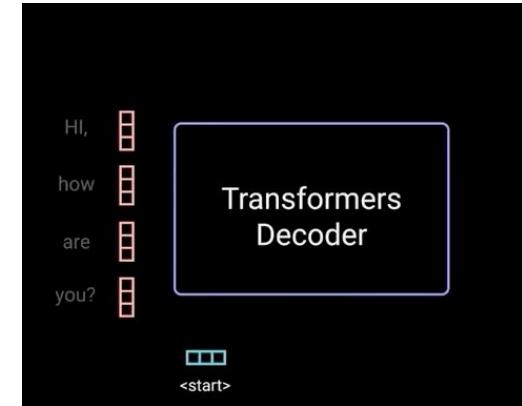


- <https://arxiv.org/abs/2405.03680> (J. Phys. Chem. Lett.)
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AtomGPT



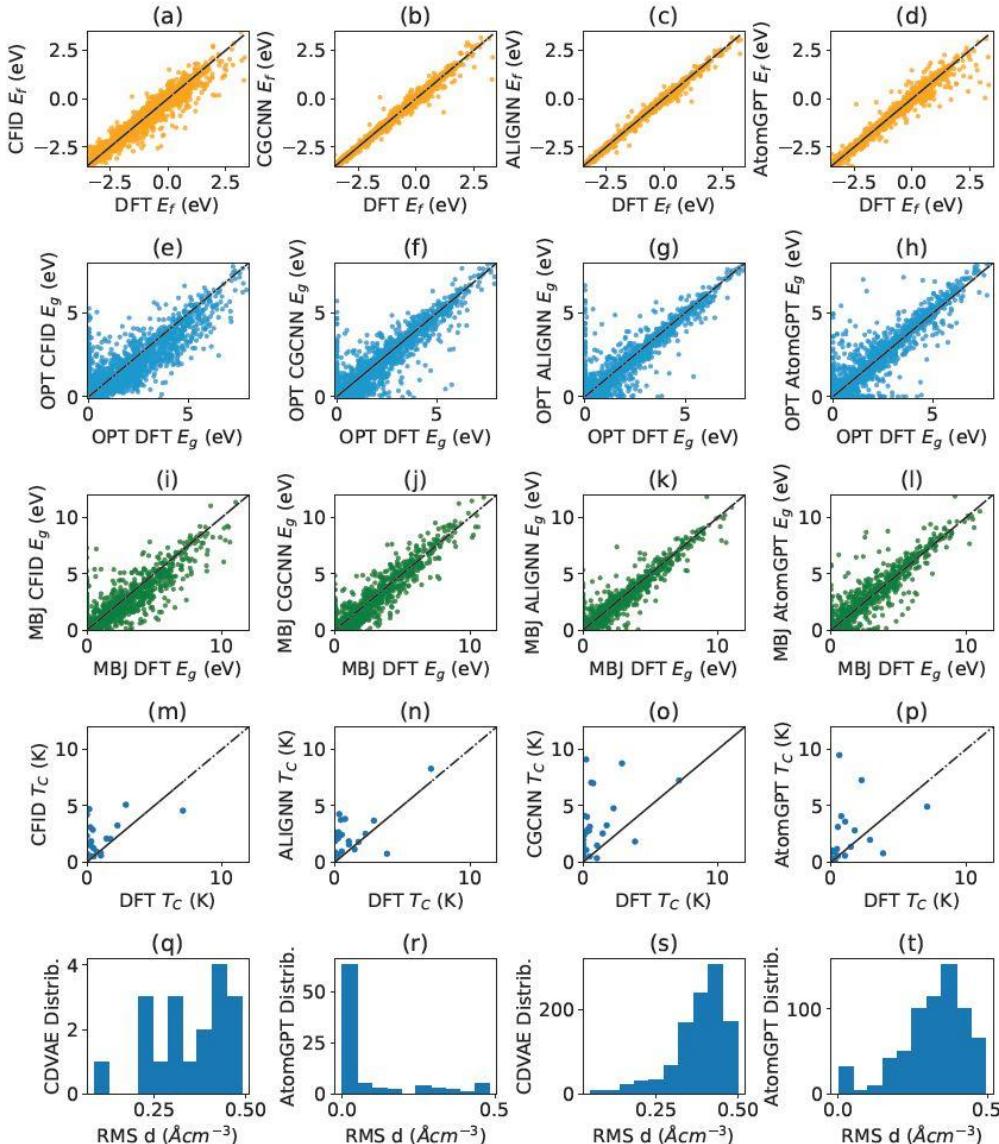
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$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$



- 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	ALIGNNN	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	0.24	0.08		
Carbon24	0.36	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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Article Views

Altmetric

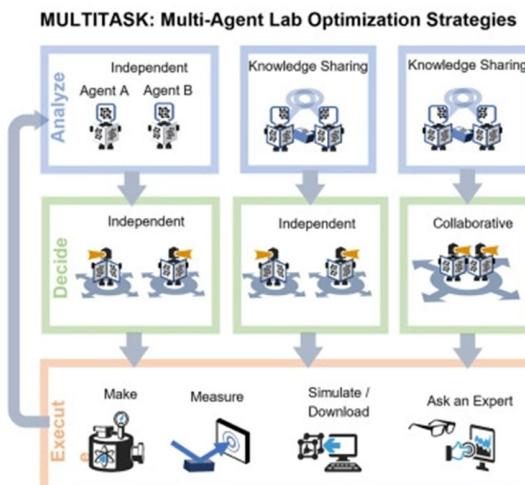
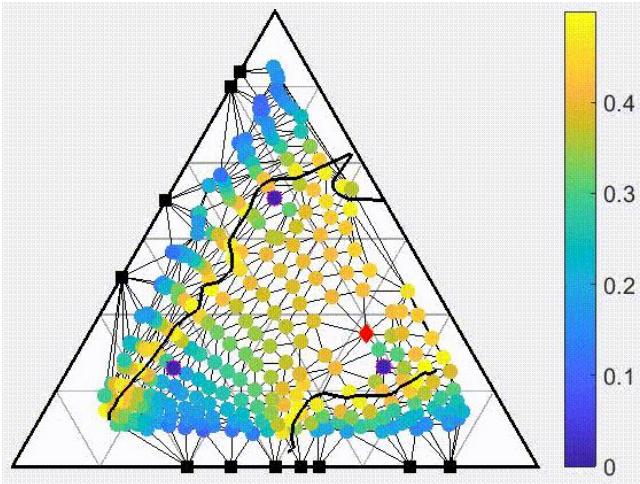
Citations

LEARN ABOUT THESE METRICS



Generated structures relaxed with ALIGNNN-FF before DFT-superconductivity workflow

Projects



◆ Autonomous Methods:

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

◆ 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

Postdoctoral Opportunities

NRC Postdoc
Opportunities:

Many project opportunities
for recent PhDs interested
in quantum materials,
machine learning,
computation, and materials
design.

- Open to U.S. citizens
- Proposal deadlines:
Feb. 1st and Aug. 1st

Our team and Collaboration



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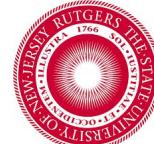
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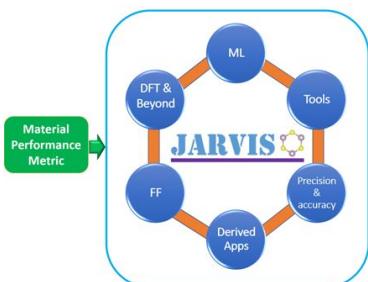
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Conclusion and Contact Information



- NIST-JARVIS is a comprehensive database and toolset for materials science research
- A one-stop resource for materials design and discovery
- It is not just a tool—it's a collaborative platform
- Thank you for your time. If you're interested in learning more or collaborating, please feel free to reach out!



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Slides: https://github.com/usnistgov/aims2024_workshop