JOHNS HOPKINS
APPLIED PHYSICS LABORATORY

Targeted AI-Driven Materials Discovery

2024 Artificial Intelligence for Materials Science (AIMS) Workshop

July 17th, 2024

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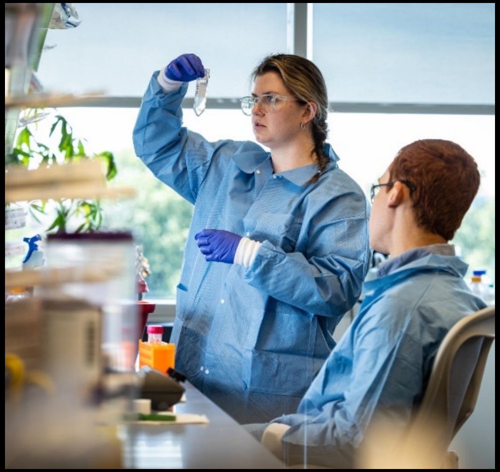
Research and Exploratory Development Department
Johns Hopkins University Applied Physics Laboratory

APL in Brief

What are we?

- Research division of Johns Hopkins University
- University Affiliated Research Center



Who are we?

- Technically skilled and operationally oriented
- Objective and independent

Who are our sponsors?

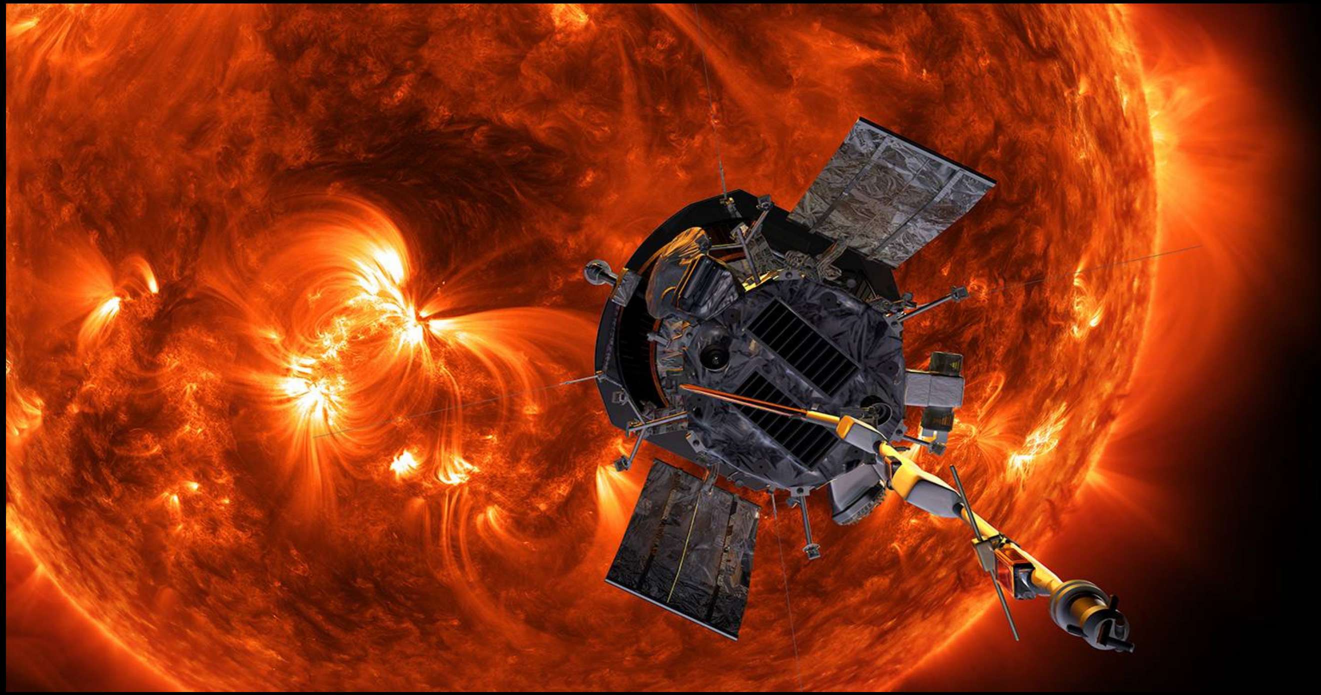
- Department of Defense
- NASA
- Department of Homeland Security
- Intelligence Community

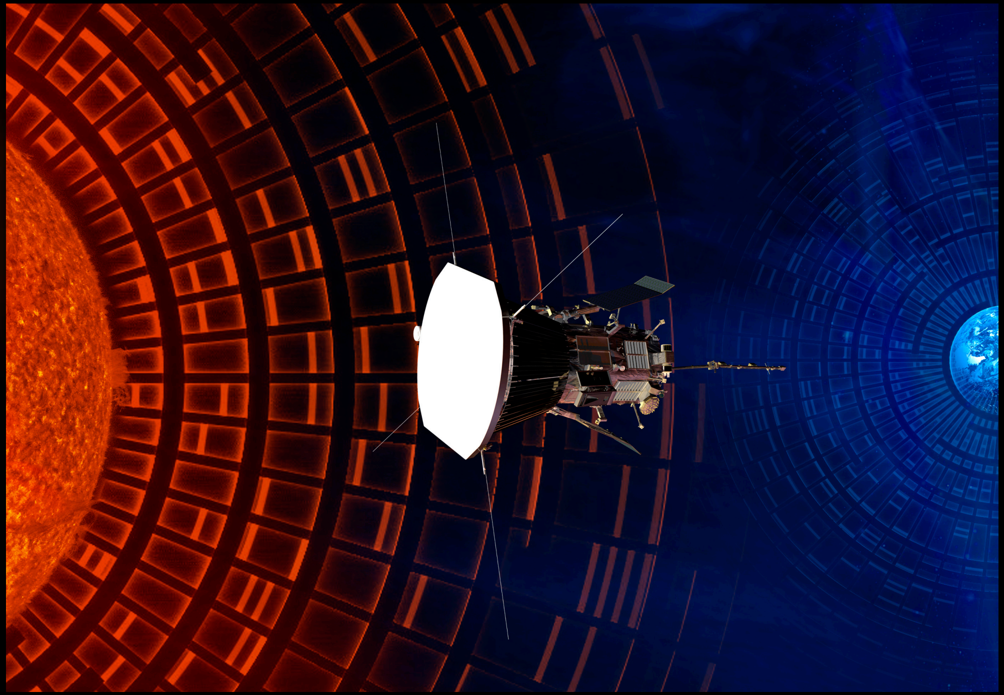
What is our purpose?

- Critical contributions to critical challenges

Pioneering Research with Mission Intent

- Understand critical mission challenge
- Assemble world-class expertise
- Conduct pioneering research
- Seek technology transition





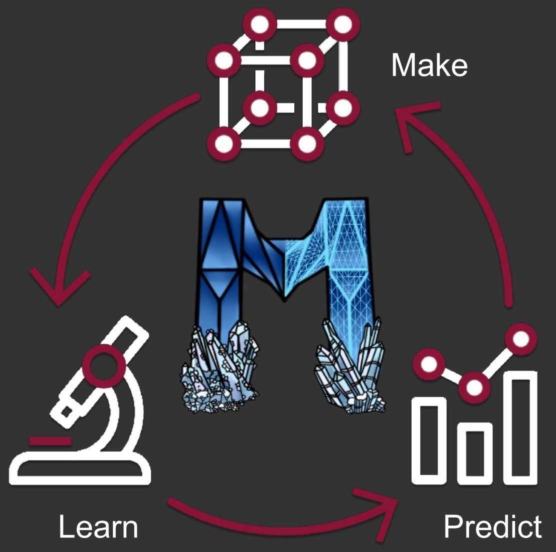
https://www.nasa.gov/content/goddard/parker-solar-probe

AI-Driven Materials Discovery

MITHRIL: *Material Invention Through Hypothesis-agnostic, Real-time, Interdisciplinary Learning*

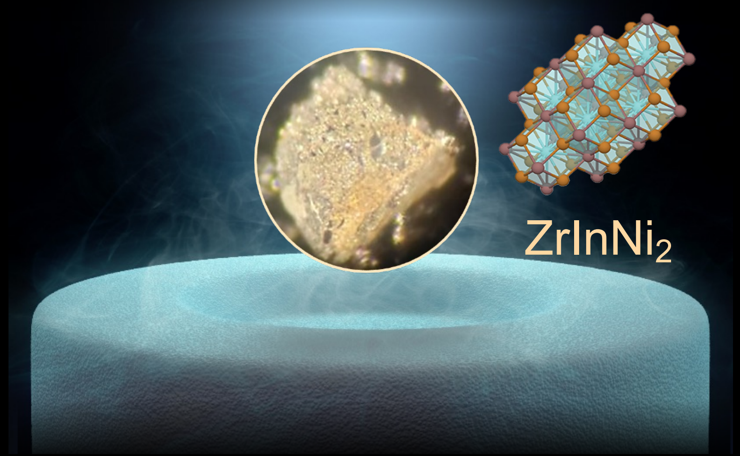
Challenge:
Accelerate the discovery of new high temperature superconductors that are manufacturable

Research:
Connect materials science, chemistry and machine learning iteratively to accelerate targeted materials discovery, design, and synthesis



Materials Discovery Cycle
PREDICT, MAKE, LEARN

MITHRIL Accomplishments
- 3 novel candidate compositions discovered
- 1 verified novel superconductor
- Advances in AI-generated structures
- Accelerated experimental data analysis
- High throughput fabrication, characterization



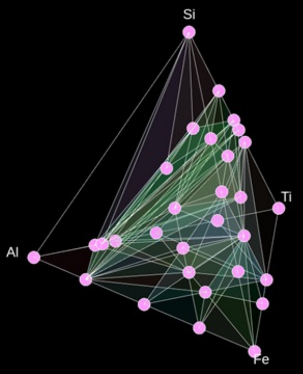
Accelerated discovery of new materials with mission-enabling properties, which could be adapted for *power transport, motors, magnets, materials discovery with constrained resources etc.*

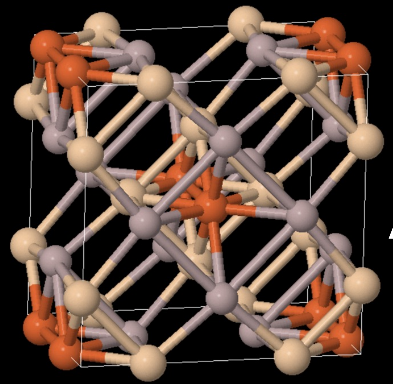
In collaboration with Professor Tyrel McQueen (JHU)

*Pogue, Elizabeth A., et al. "Closed-loop superconducting materials discovery." npj Computational Materials 9.1 (2023): 181.

Materials Discovery is a Triple Problem

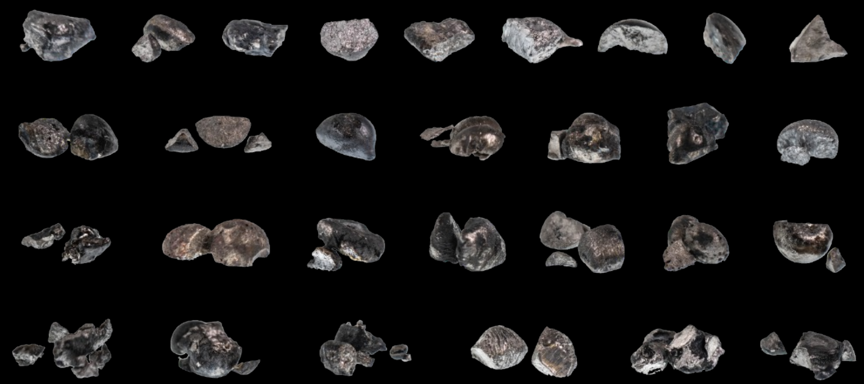
Theoretic Discovery



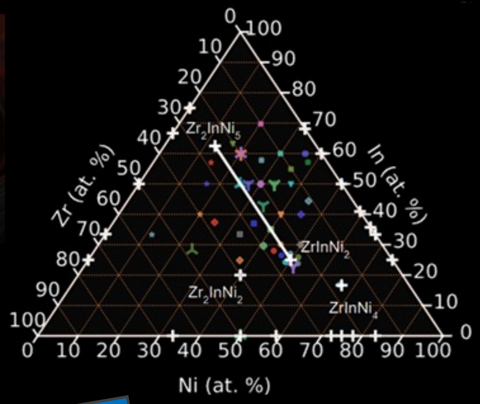


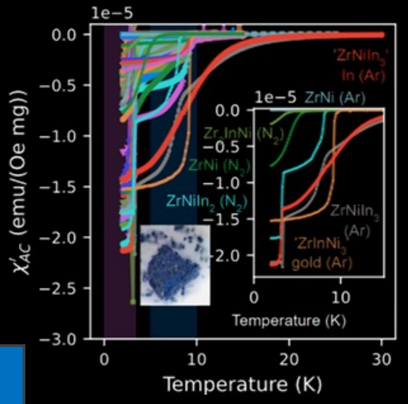
Al_2FeSi_2
$I4/mmm$

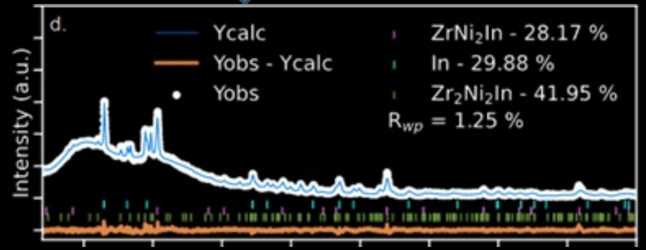
Synthesis Discovery



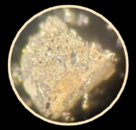
Verification of Discovery







$ZrInNi_2$



AI-Driven Materials Discovery on the Lunar Surface

ELEM3NT Discovery: Enabling a Lunar Ecosystem via Materials Modeling & Manufacturing Novelty & Throughput-based Discovery

- **Problem**
  - Leverage LLMs to generate lunar material and synthesis knowledgebases
  - Incorporate mission-constraints in AI-guided resource utilization pipeline
- **Prediction**
  - Generate stable candidate materials via physics-based models
  - Incorporate understanding of process-property relationships
- **Production**
  - Create novel materials utilizing high throughput fabrication
  - Characterize materials with an efficient hierarchy of high-throughput characterization

in-situ Constrained Materials Discovery

Oxide	Avg. Apollo 16 soil
SiO_2	45.0
TiO_2	0.54
Al_2O_3	27.3
Cr_2O_3	0.33
FeO	5.1
MnO	0.30
MgO	5.7
CaO	15.7
Na_2O	0.46
K_2O	0.17
P_2O_3	0.11
S	0.07

Challenging Materials Requirements

- Pressurized spaces 10^5 Pa (15 psi)
- Large temperature variations and gradients
- Radiation environment
- Micrometeorite impacts

Source: NASA https://moon.nasa.gov/observe-the-moon-night/resources/moon-map/

From Data to Knowledge

LunaGPT: Envisioned Partnership

Creation of a dynamic, queryable knowledge base of lunar materials

Information Retrieval

“What trace elements can be found at the South Ray Crater?”

Al, Si, O, Fe, Ti, Cr, Mg, Mn, Ca, Na

Extrapolation

“What materials do you think might be available across the Moon?”

Synthesis Planning

“Where and what steps should I take in order to synthesize microstructure X from AlO_2?”

From Data to Knowledge

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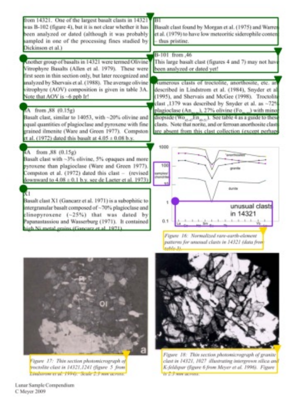
Pre-processing:
CHOMP: Domain-informed, content-aware LLM parses and classifies



Retrieval

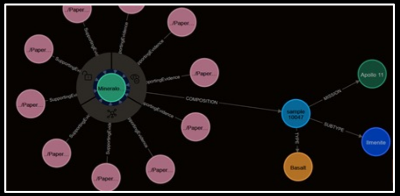
700+ documents[1] and counting!

Contextualization
- Preserved relationships
- Traceability
- Improved accuracy

Query

Domain-Informed Response

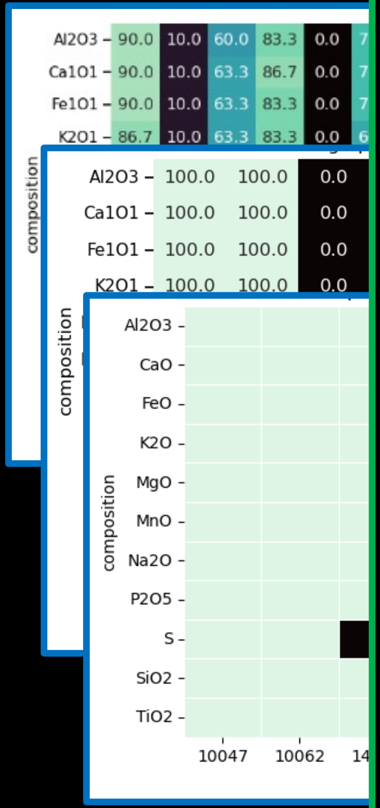
Indexed Vector Representations + Graph Networks

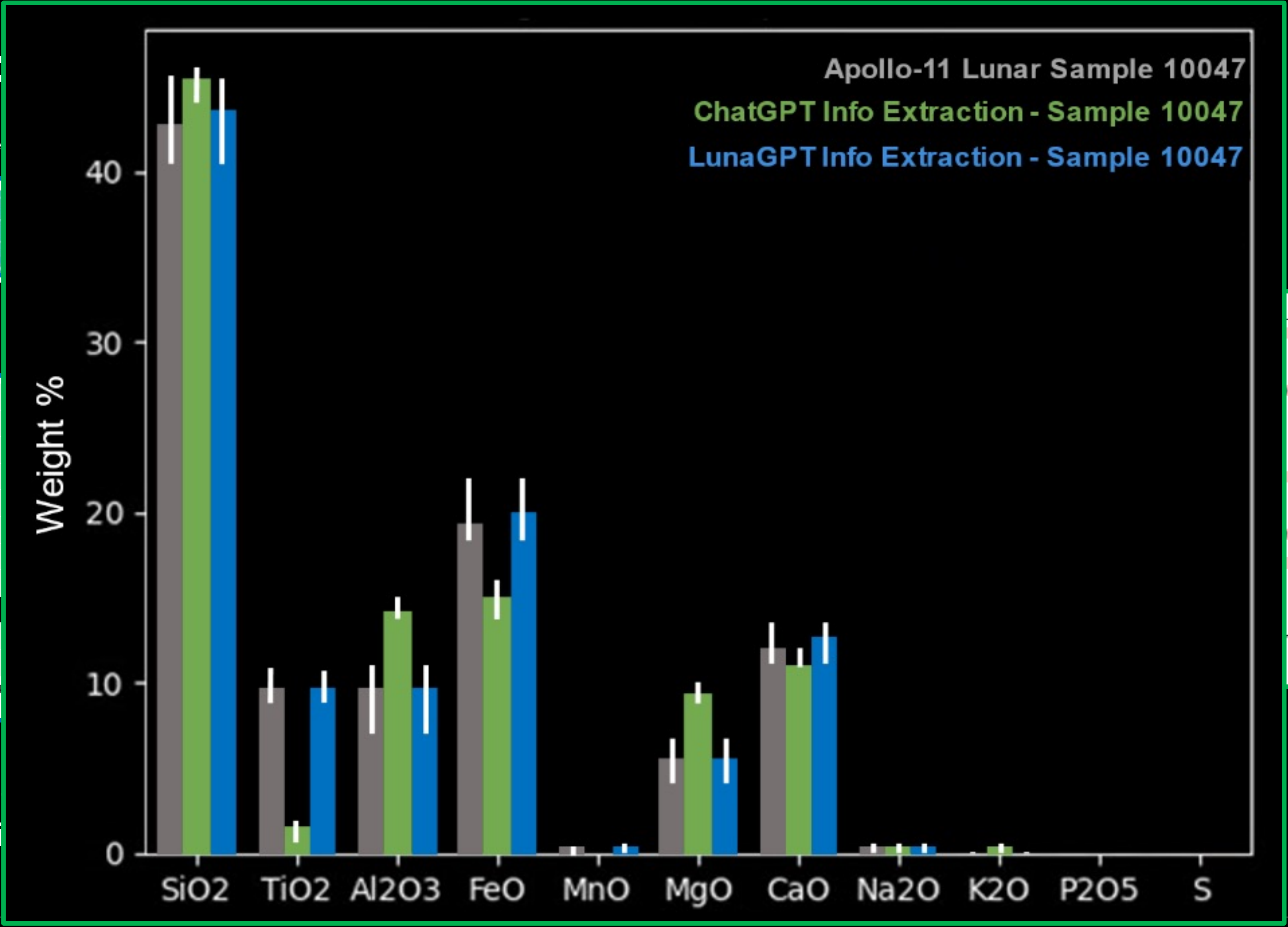


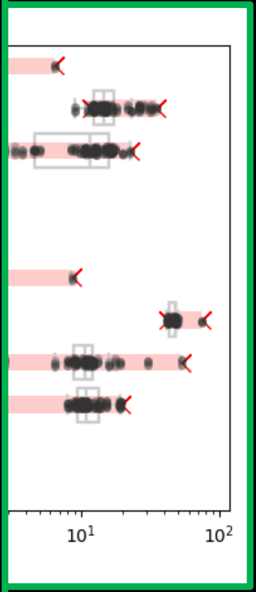
‘Intelligent’ Retrieval Augmented Generation

LunaGP

Per-oxide







Evaluation

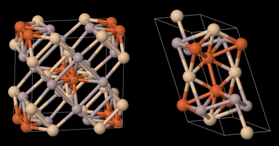
extraction

compositi

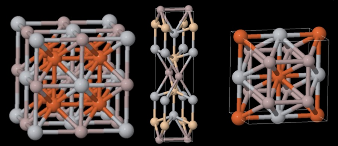
Material Candidate Pipeline

Only: Al, Si, O, Fe, Ti, Cr, Mg, Mn, Ca, Na

Designing Lunar Structural Materials



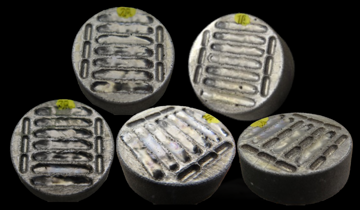
~10^6 crystal structures generated with PGCGM[2] and CDVAE[3]

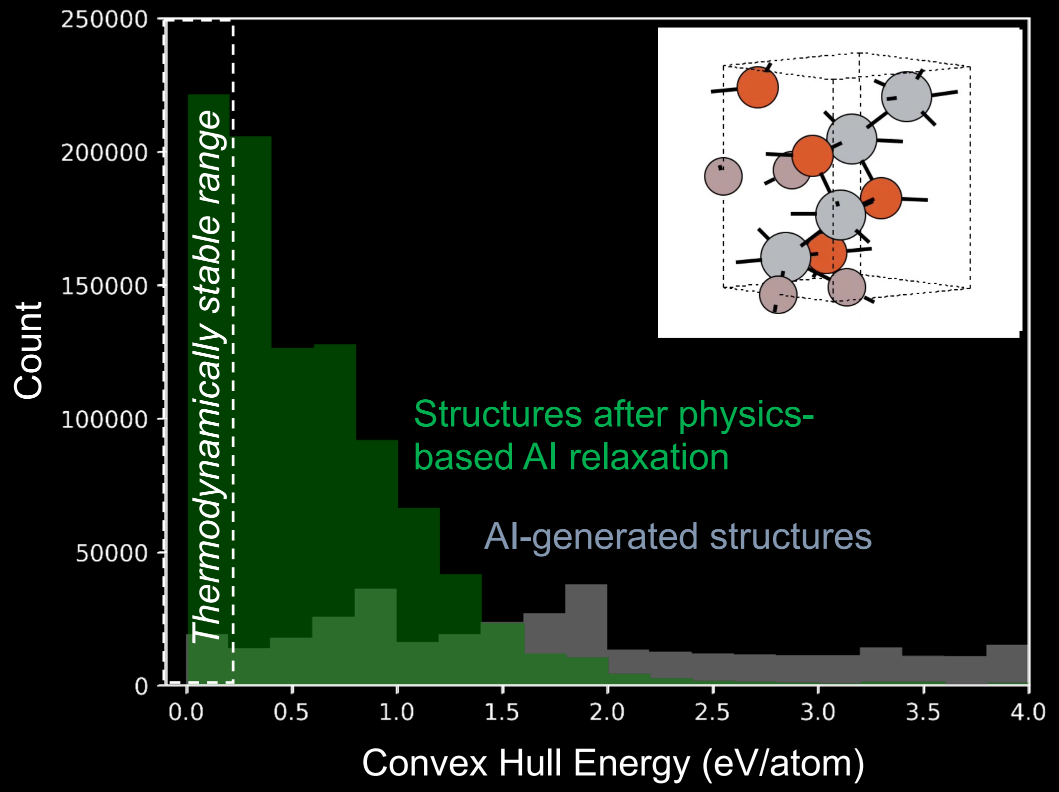


Structures relaxed → Stability of candidates estimated with CHGNET

ML mechanical property predictions implemented as additional filter

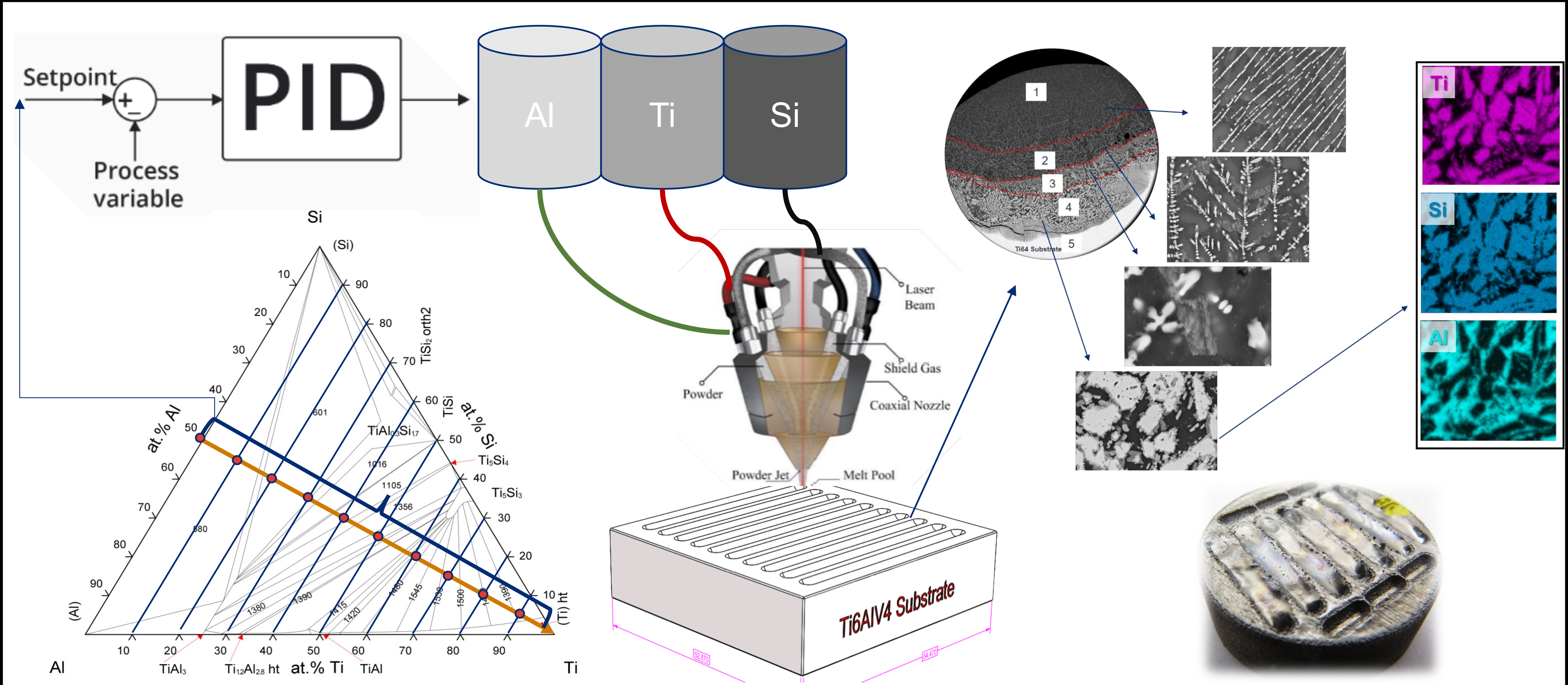
Synthesis and characterization of 100s of compositions



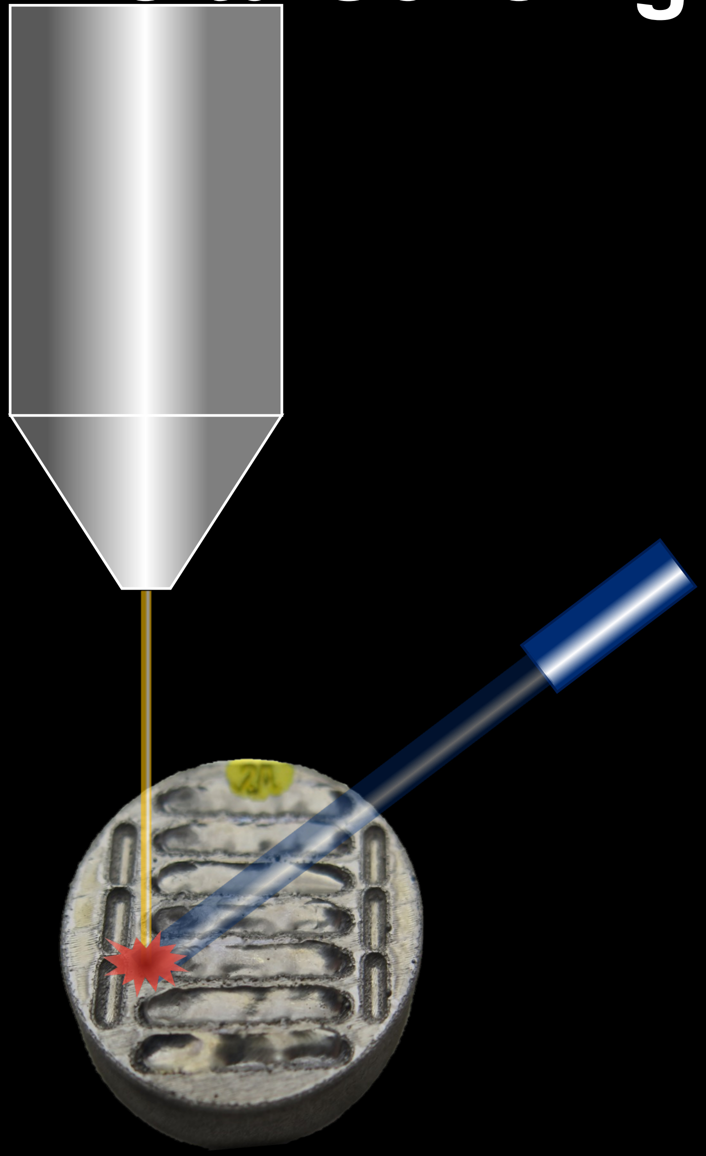


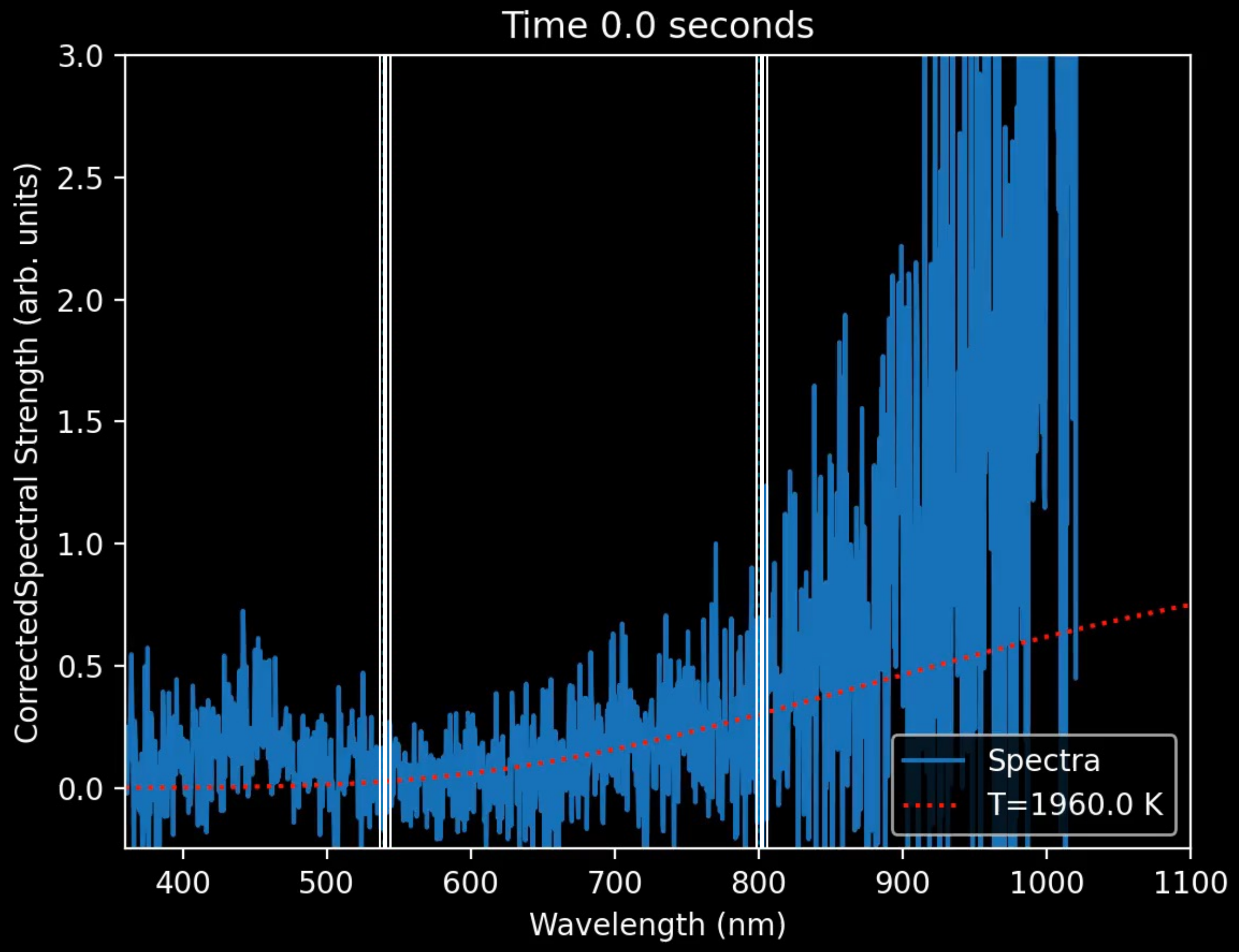
[1] New, A. et al. "Evaluating the diversity and utility of materials proposed by generative models," ICML S&S 2023 https://openreview.net/forum?id=2ZYbmYTKoR
[2] Zhao, Y., et al. Physics guided deep learning for generative design of crystal materials with symmetry constraints. npj Comput Mater 9, 38 (2023).
[3] Xie, Tian, et al. "Crystal diffusion variational autoencoder for periodic material generation." arXiv preprint arXiv:2110.06197 (2021).

Directed Energy Deposition Synthesis



in-situ Sensing During Synthesis





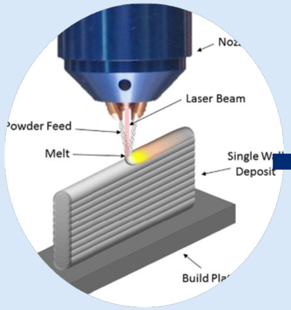
Strong Spectral Emissions (Chemical Information)

Temperature Fitting Region

Saturated From Laser

Efficient, High Throughput Characterization and Data Gen.

Performed on All Samples



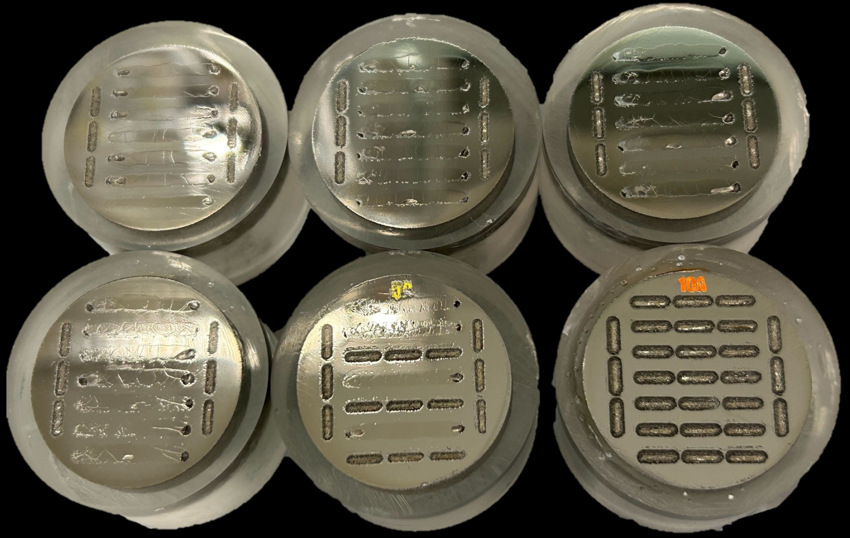
XRF for composition → (Roughly section) → XRD for structure

Performed on Some Samples (requires polishing)

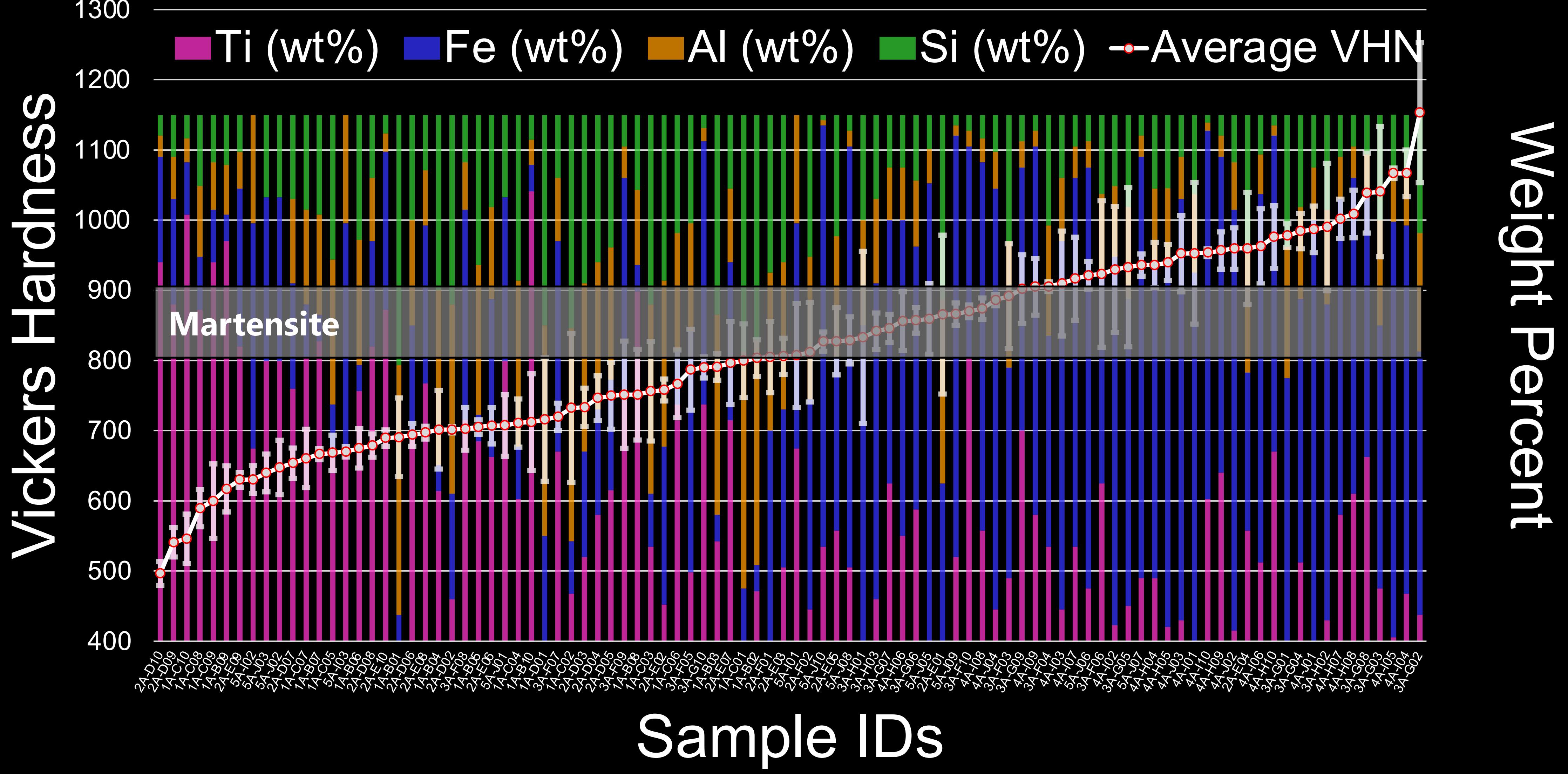
- Nanoindentation for hardness
- Nanoindentation for yield?
- EDS and SEM for microstructure
- µCT for impurity distribution, porosity

Performed on Very Few, Targeted Samples (precise geometries)

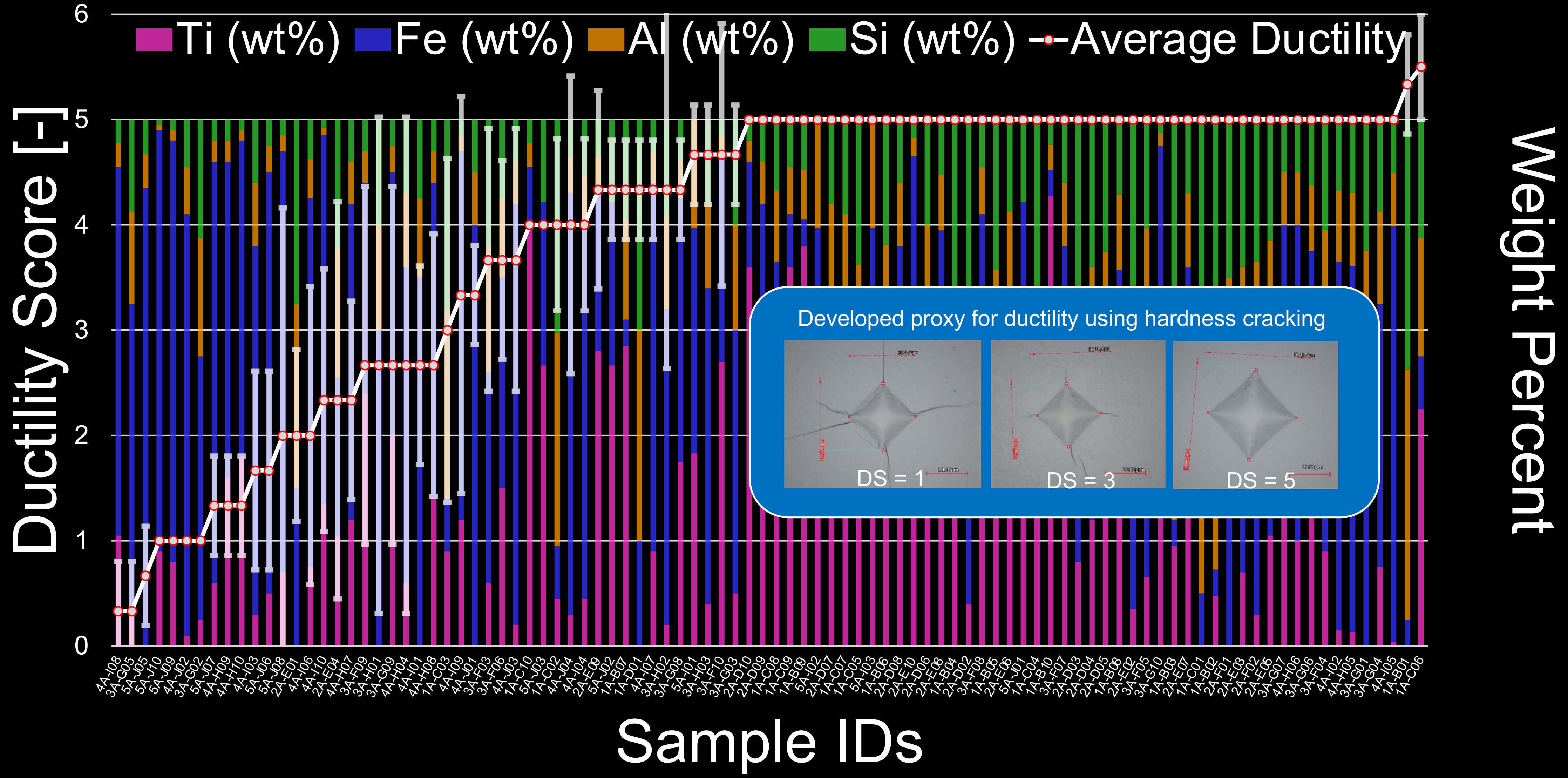
- Tensile Tests
- Thermal Conductivity
- Model fabrication of real shapes
- Other



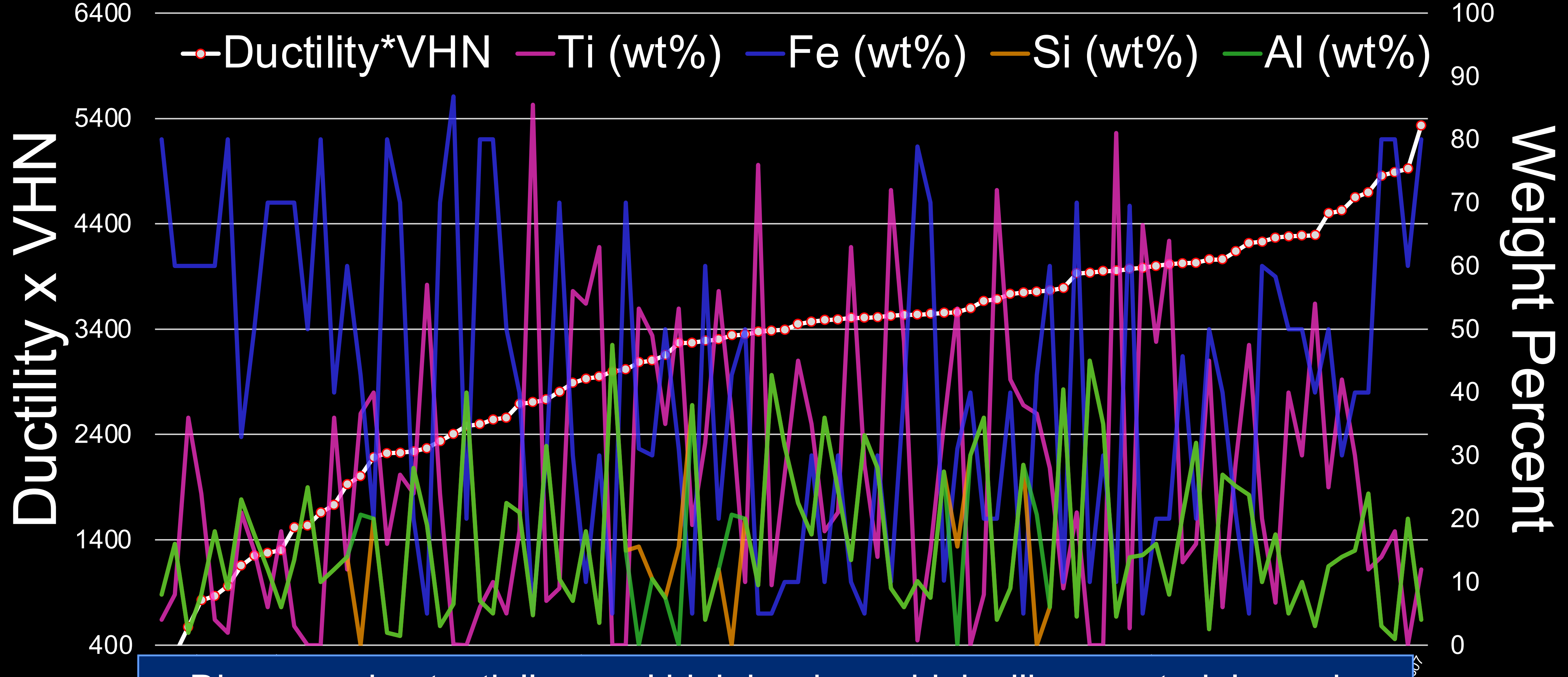
Insights and Potential Discoveries



Insights and Potential Discoveries

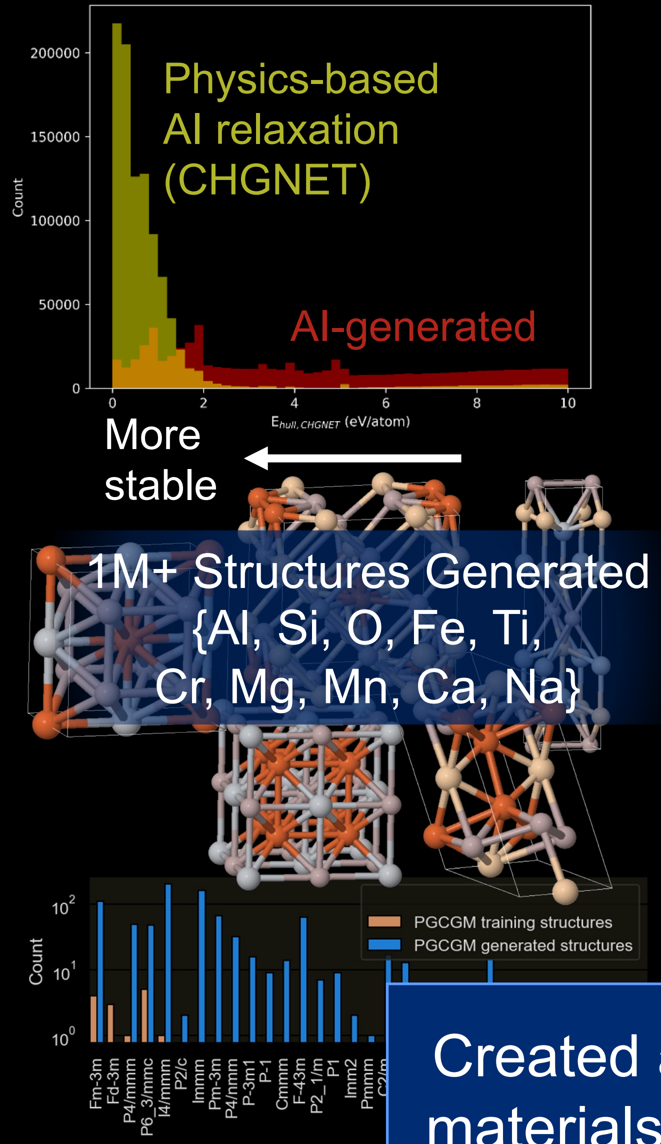


Insights and Potential Discoveries

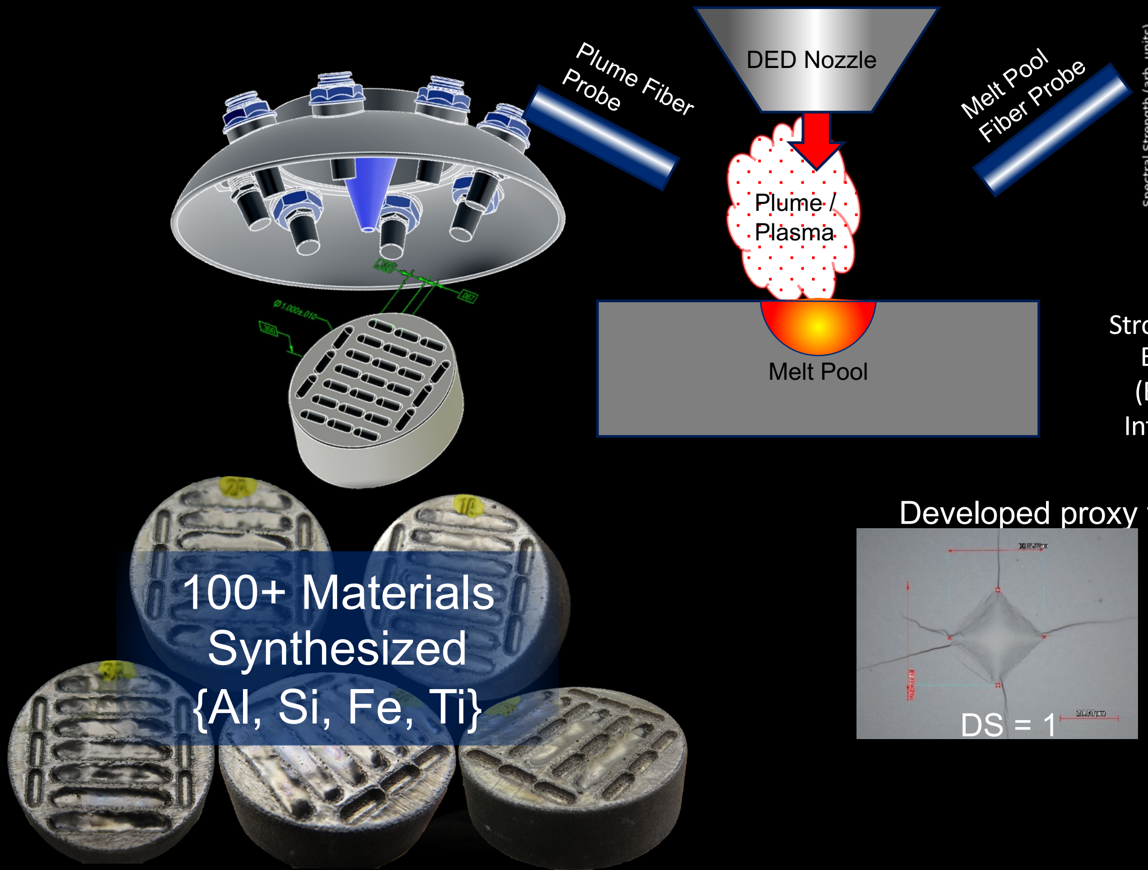


Discovered potentially novel high hardness high silicon materials made from elements that can be found on the Moon in abundance (Fe, Al, Ti, Si)
Characterization in progress at JHU

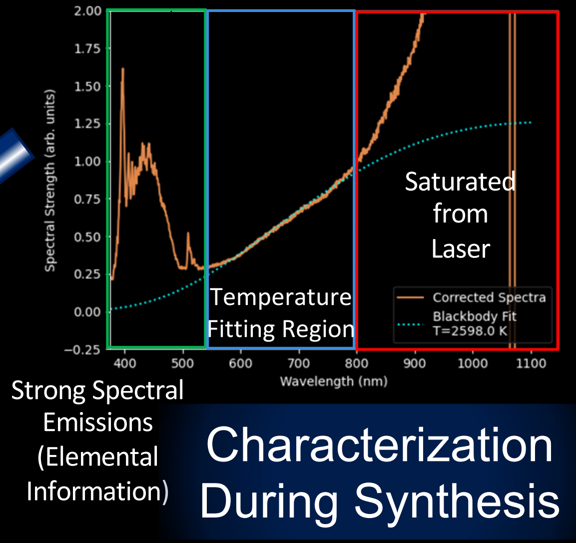
Predict



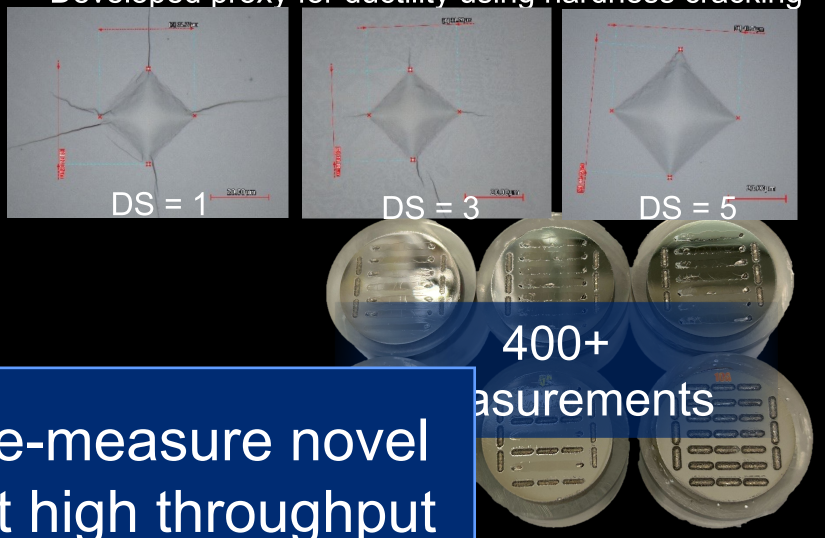
Make



Measure



Developed proxy for ductility using hardness cracking



Created an AI-Guided pipeline to predict-make-measure novel materials utilizing primarily in-situ resources at high throughput

Takeaways

Summary:

- LunaGPT - created extensive lunar materials knowledgebase that is dynamically queryable
- Predict-make-measure novel materials utilizing primarily in-situ resources at high throughput
- Discovered new high hardness high silicon materials made from elements that can be found on the Moon in abundance (Fe, Al, Ti, Si)

Conclusions:

- Closed-loop machine learning, combining prediction, experimental validation and feedback, can greatly accelerate the intentional discovery of novel materials with target properties, even without full knowledge of the underlying physics
- This closed-loop approach is applicable to other material domains
- Current opensource generative models like are able to generate large numbers of varied and valid material structures (with help)
- There are many places to innovate in AI accelerated closed loop materials discovery

Future Needs:

- Techniques that go beyond ternary phase generation and defects/synthesis related descriptors are needed
- Extend materials representations in AI/ML models to capture intricate physics (defects, dopants, interfaces,…)
- AI-guided synthesis pathway prediction

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The ELEM3NT Discovery Team


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In collaboration with the:

Tyrel M. McQueen Group at JHU; Brandon Wilfong, Gregory Bassen, Elisabeth Hedrick

Mark Foster Group at JHU; Collin Goodman

Upcoming JHU/APL Symposium

September 5, 2024 at JHU/APL in Laurel, MD

https://secwww.jhuapl.edu/EventLink/Event/384

Visit the site to learn more & register!

TOPICS:

- AI-Driven Material Discovery
- Materials Design and Simulation
- High-Throughput Fabrication and Testing
- Data-Driven Insights
- Challenges and Opportunities

Speakers & Panelists from Govt, Industry & Academia

Thank you for your attention

JHU/APL
Materials Research

← See our papers:

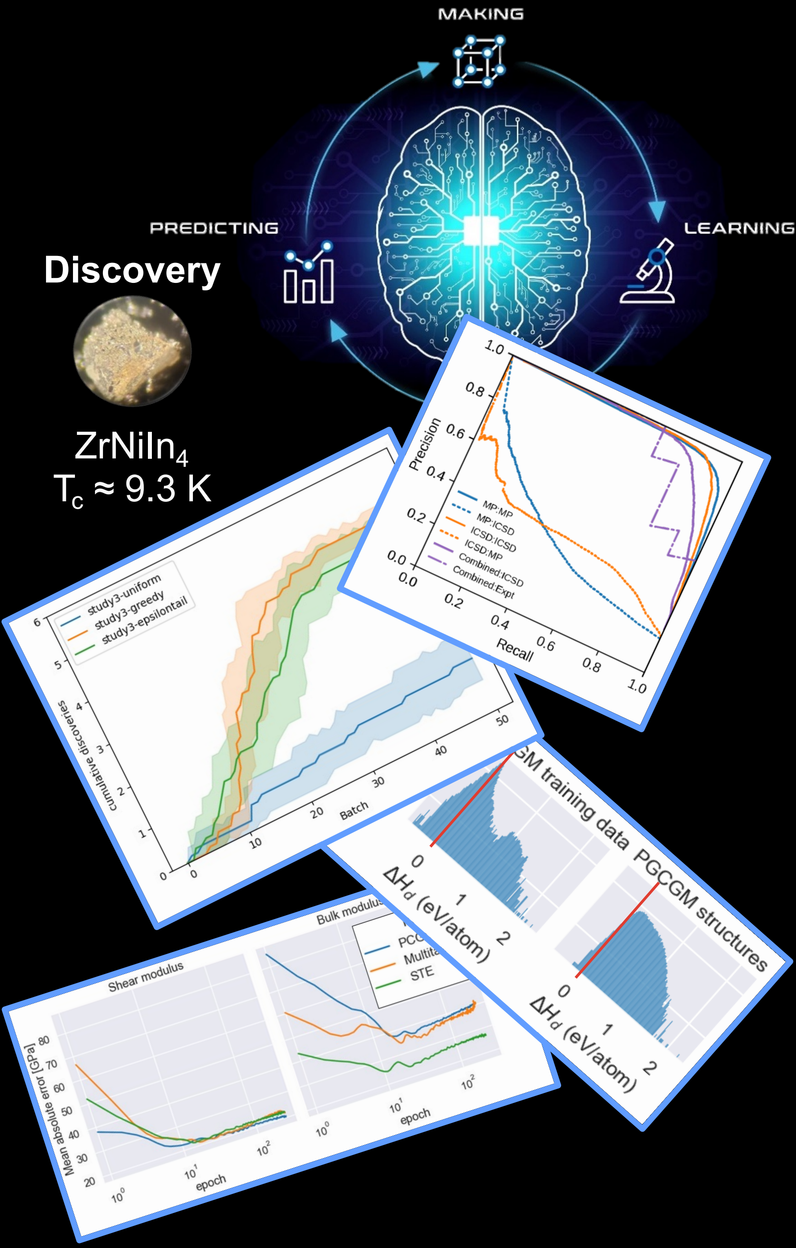
"Closed-loop Superconducting Materials Discovery," Pogue, E. A., New, A., McElroy, K., Le, N. Q., Pekala, M. J., McCue, I., ... & Stiles, C. D., npj Computational Materials, 9, 181 (2023) https://doi.org/10.1038/s41524-023-01131-3

"Evaluating the diversity and utility of materials proposed by generative models," New, A., Pekala, M., Pogue, E. A., Le, N. Q., Domenico, J., Piatko, C. D., & Stiles, C. D., 1st Workshop on the Synergy of Scientific and Machine Learning Modeling @ ICML2023 https://arxiv.org/abs/2309.12323

"Deep Learning Models to Identify Common Phases across Material Systems from X-ray Diffraction," Le, N. Q., Pekala, M., New, A., Gienger, E. B., Chung, C., Montalbano, T. J., ... & Stiles, C. D., The Journal of Physical Chemistry C, 127, 21758 (2023), https://doi.org/10.1021/acs.jpcc.3c05147

"Evaluating AI-guided Design for Scientific Discovery," Pekala, M., Pogue, E. A., New, A., Bassen, G., Domenico, J., McQueen, T. and Stiles, C. D., AI for Accelerated Materials Design - NeurIPS 2023 Workshop, https://openreview.net/pdf?id=SfEsK3O2KT

"Curvature-informed multi-task learning for graph networks," New, A., Pekala, M. J., Le, N. Q., Domenico, J., Piatko, C. D., & Stiles, C. D., AI for Science Workshop ICML2022 (2023) https://arxiv.org/abs/2208.01684



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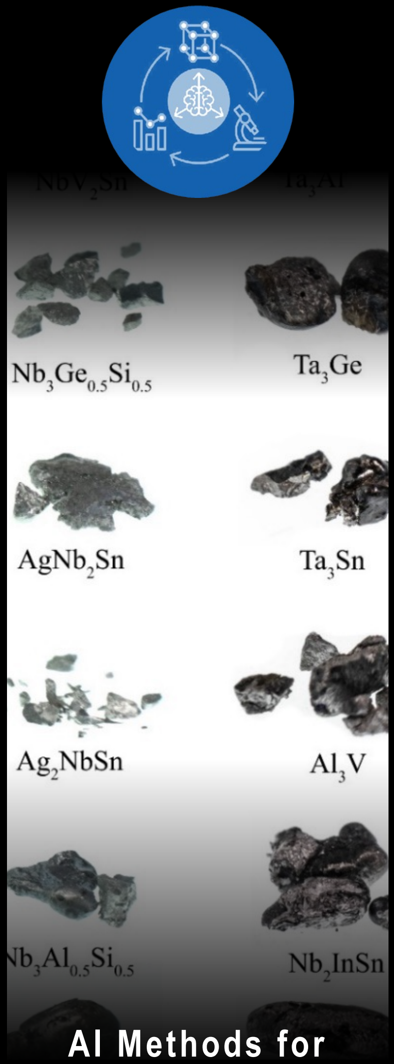
Future Vectors Connecting APL Missions

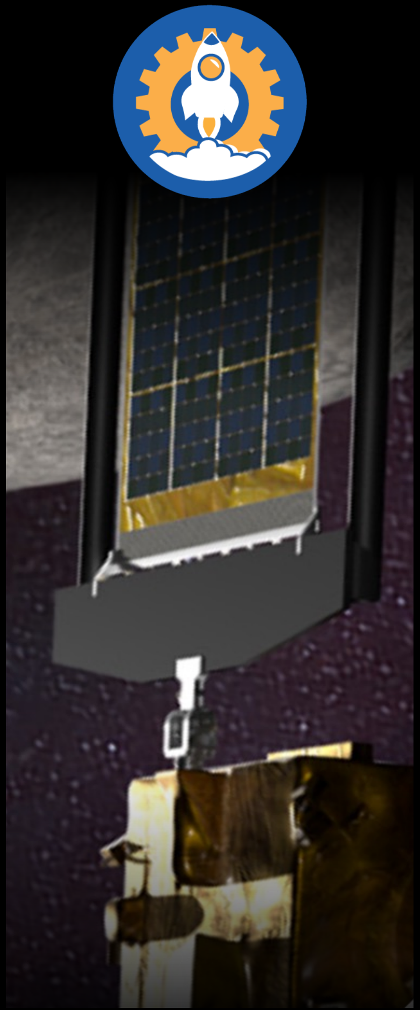


AI Methods for Materials Discovery

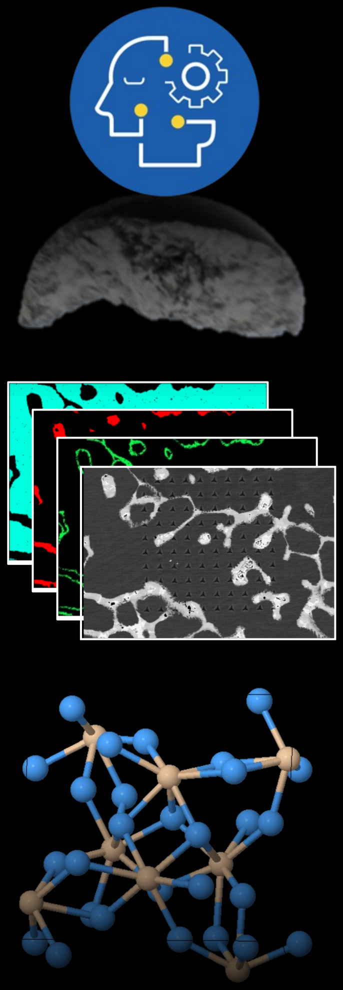
Novel Materials Characterization

In situ Resource Constraints

Synthesis & Manufacturing Pathways



Design & Task Optimization



Novel Materials & Systems Representations

Johns Hopkins

Applied Physics Laboratory