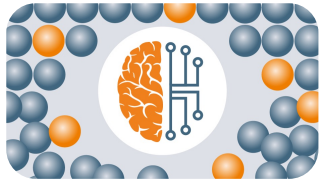
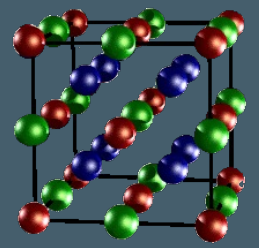


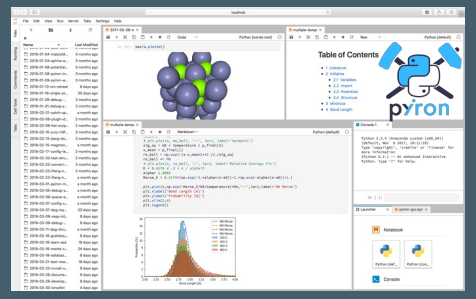
MAX PLANCK INSTITUTE
FOR SUSTAINABLE MATERIALS

Large Language Model Agents for Atomistic Simulation Workflows

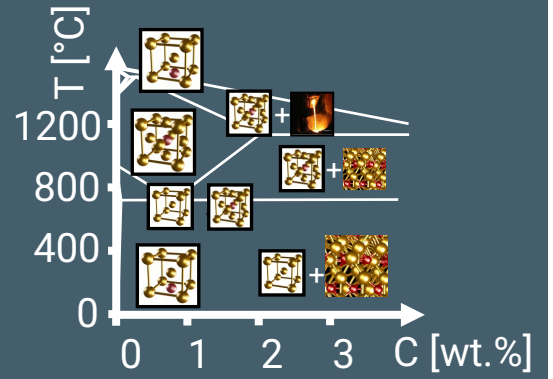
Jan Janssen – Group Leader for Materials Informatics



Simulation



Machine Learning for Workflows



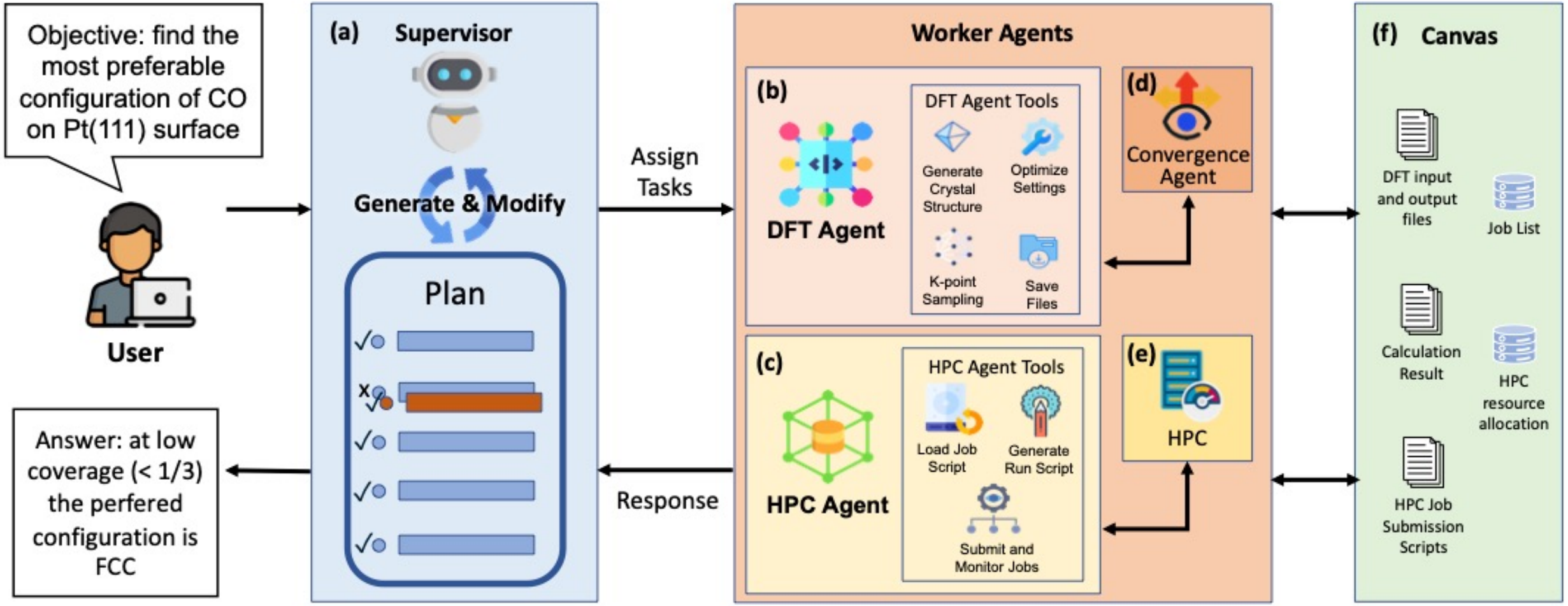
Materials Design

2026/05/20 – Workflow Community

DFT-based Research Engine for Automated Materials Screening

Collaborative Team of Large Language Model Agents

UNIVERSITY OF MICHIGAN

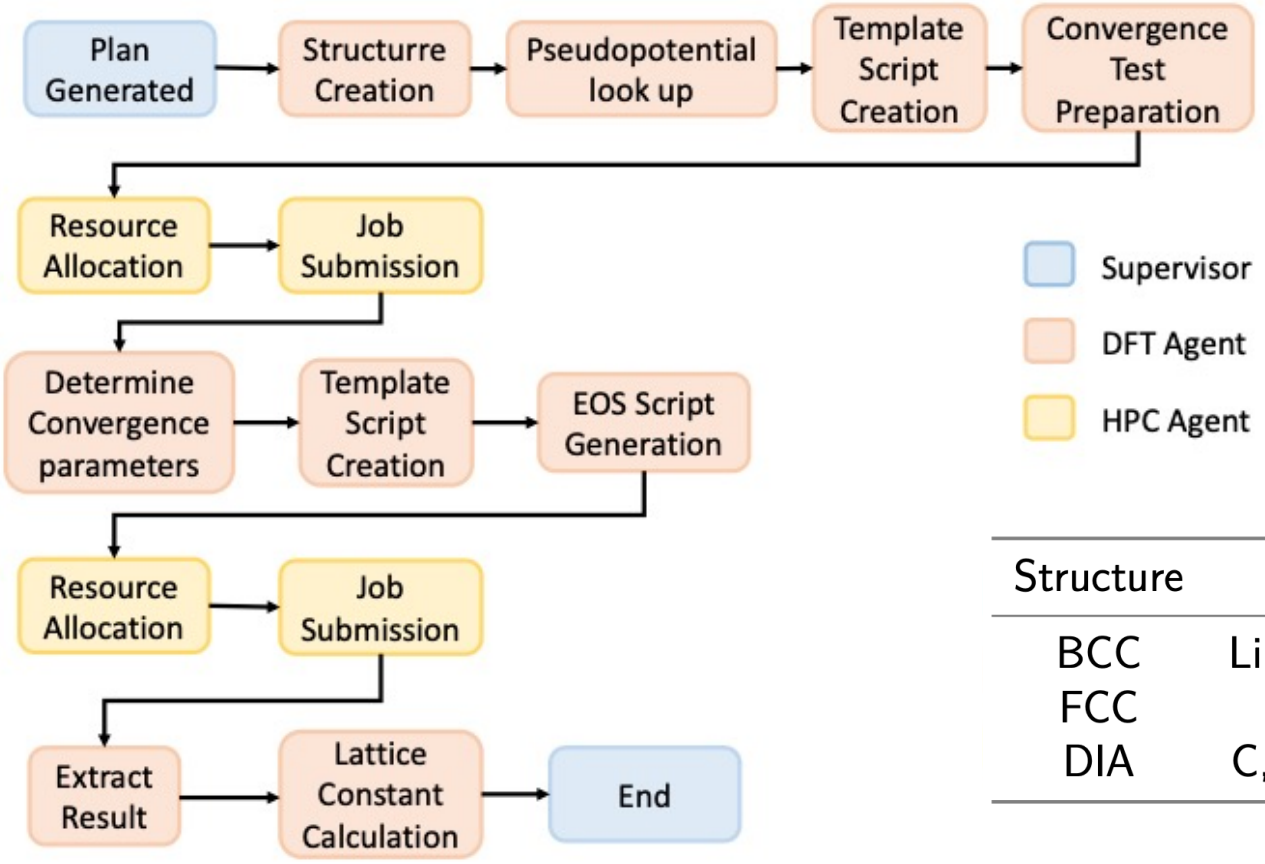


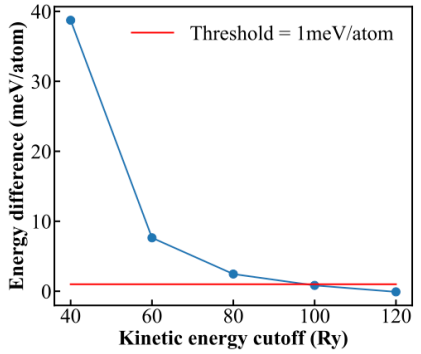
Z. Wang, H. Huang, H. Zhao, C. Xu, J. Janssen and V. Viswanathan – arXiv 2507.14267 (2025).

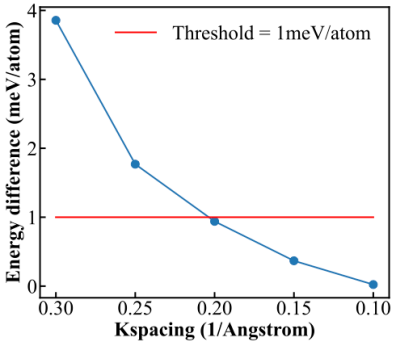
Benchmark DREAMS on the Sol27LC Benchmark

Lattice Constant Prediction

You are going to calculate the lattice constant for FCC Copper through DFT.
The experimental value is 3.6149Å; use this to create the initial structure.







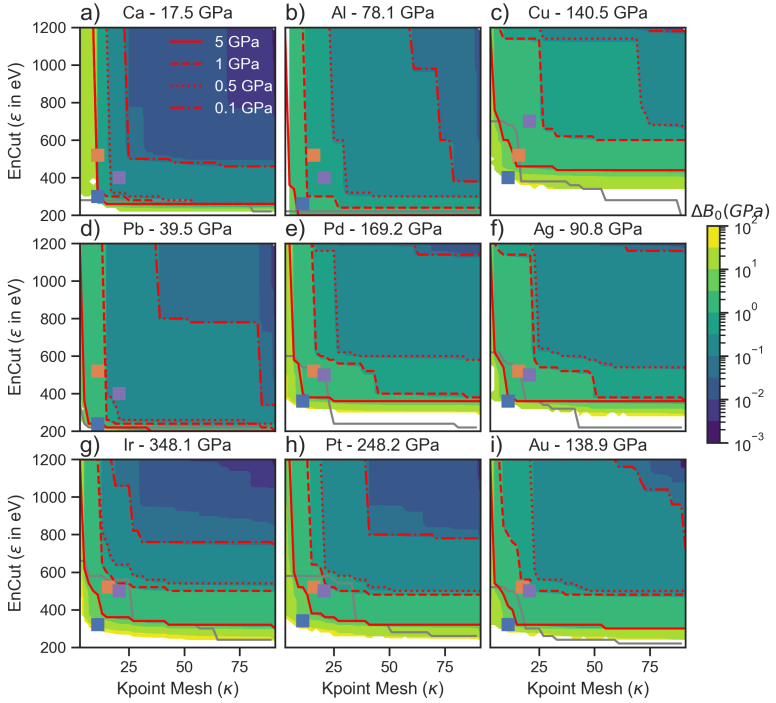
Structure	Systems	# of correct structures	MAPE
BCC	Li, Na, K, ...	11/11	**0.36%**
FCC	Rh, Ir, ...	12/12	**0.51%**
DIA	C, Si, Ge, ...	4/4	**1.00%**

Z. Wang, H. Huang, H. Zhao, C. Xu, J. Janssen and V. Viswanathan – arXiv 2507.14267 (2025).

What did we learn so far?

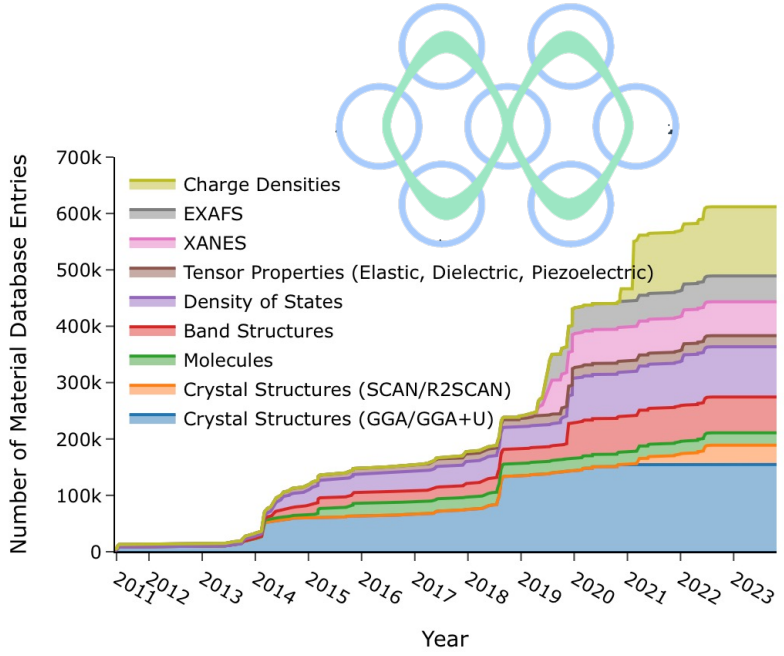
Why are Density Functional Theory LLM Agents successful?

Method Development



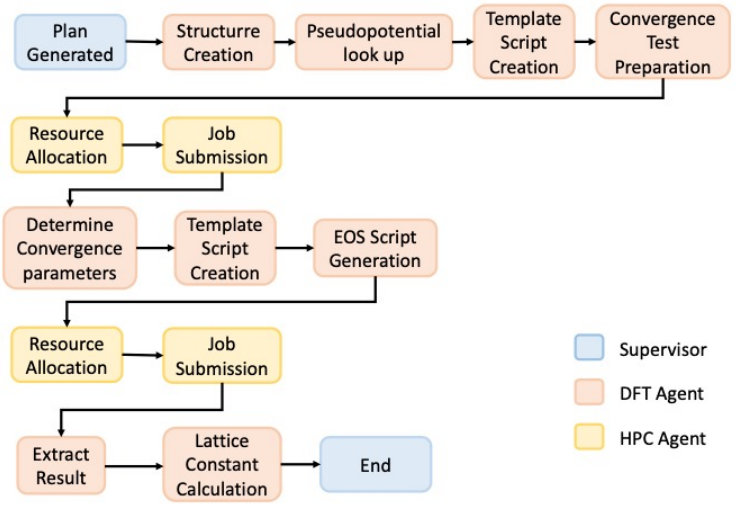
A number of methods have been developed by the community.

High Throughput Screening



A large number of software tools has been developed as part of the materials project and other high throughput screenings.

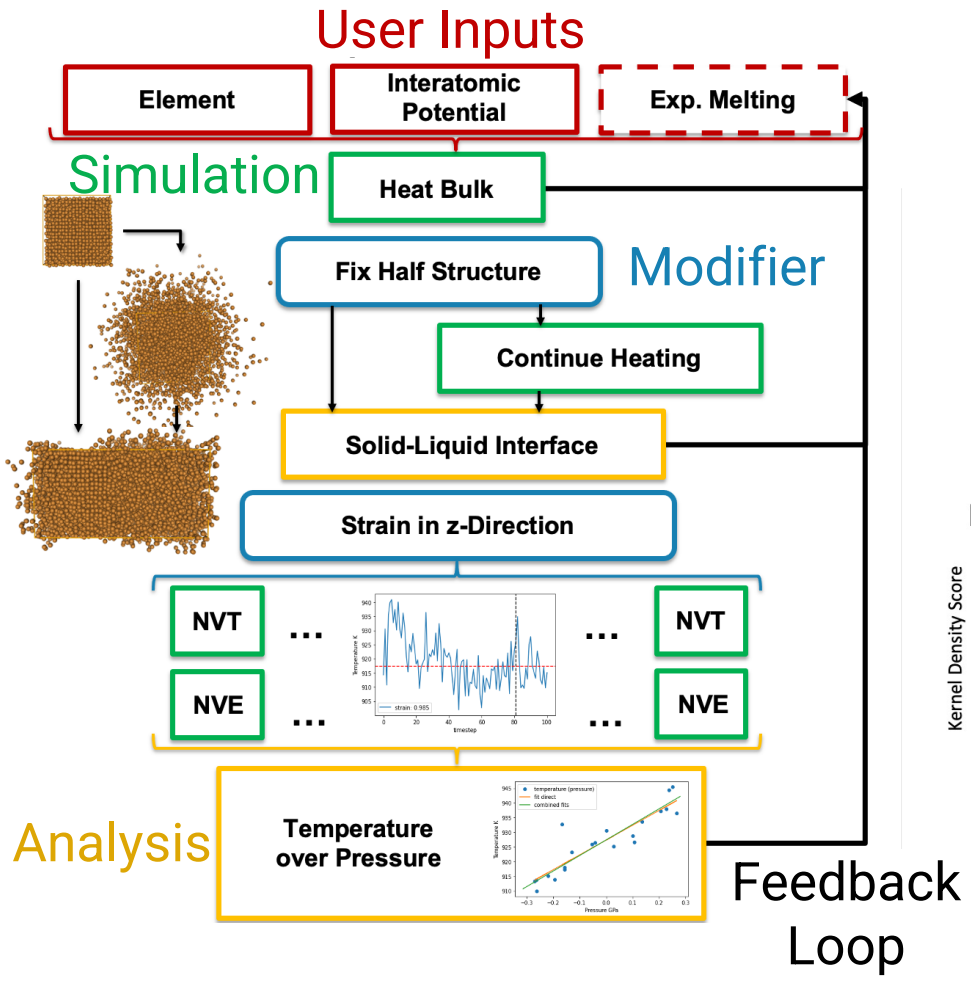
Large Language Model Agents for Quantum Mechanical Simulation



Once the methods are extended to handle all the edge cases it is save to provide them to unexperienced users.

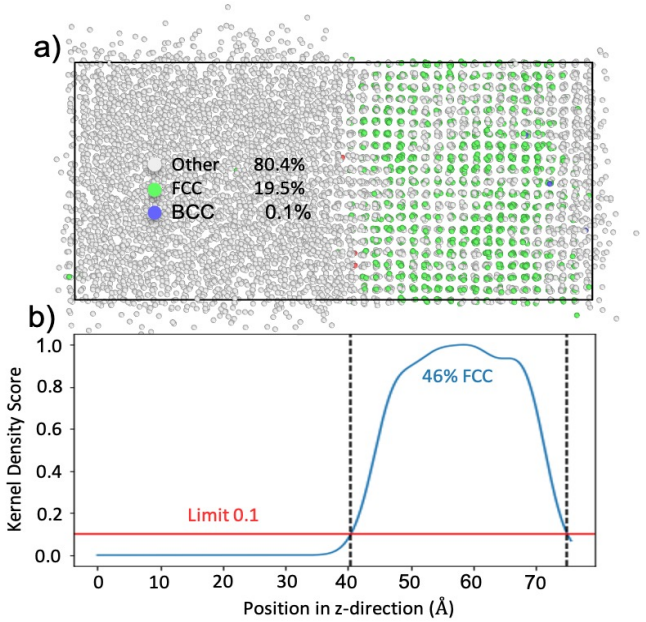
Autonomous Melting Temperature Calculation

Iterative Convergence

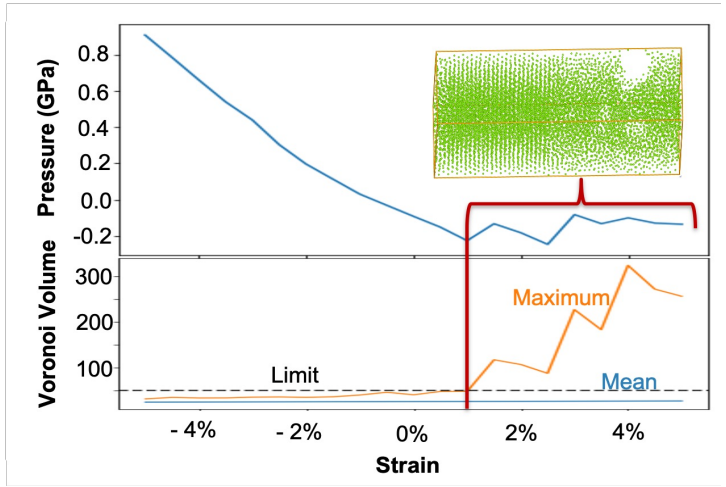


Challenges:

Solid Liquid Detector



Void Detector



L.F. Zhu, J. Janssen, et al. Comp. Mat. Sci. 187 (2021)

Autonomous Melting Temperature Calculation

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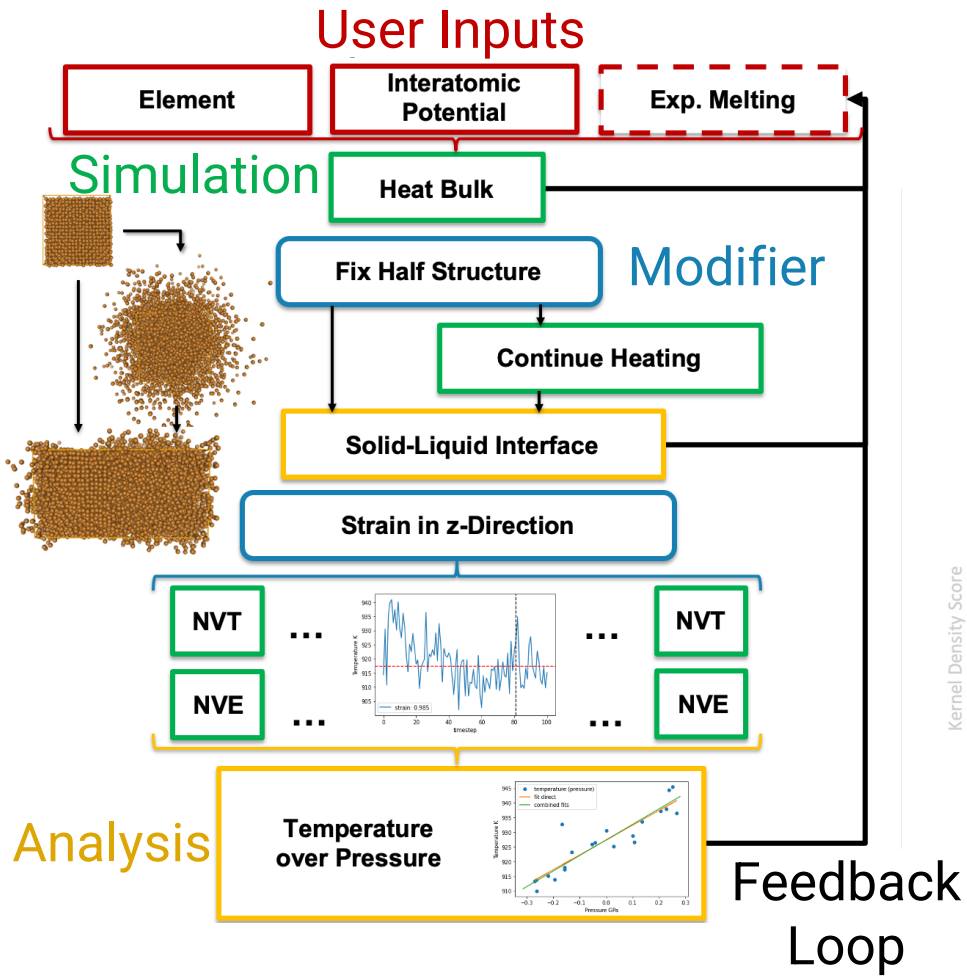
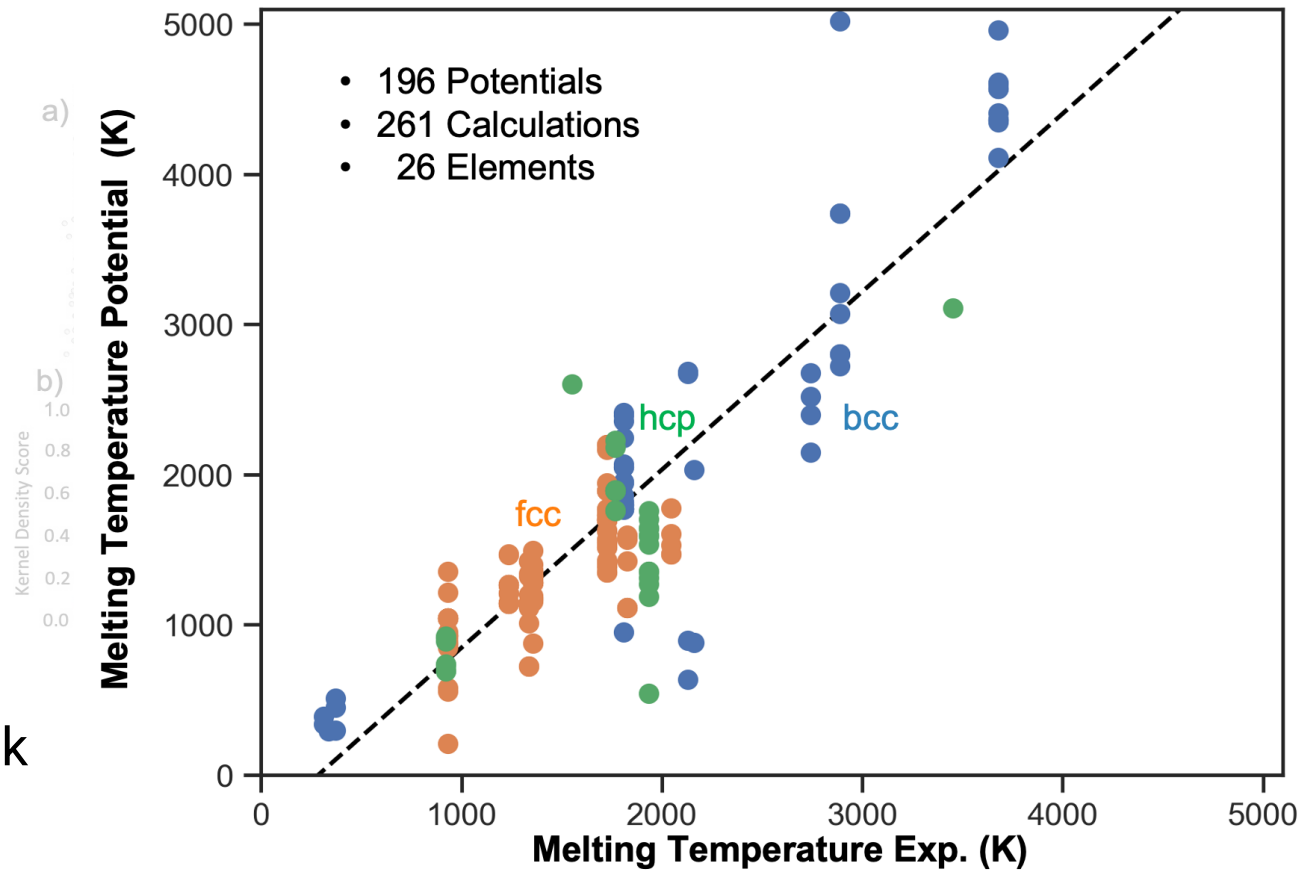


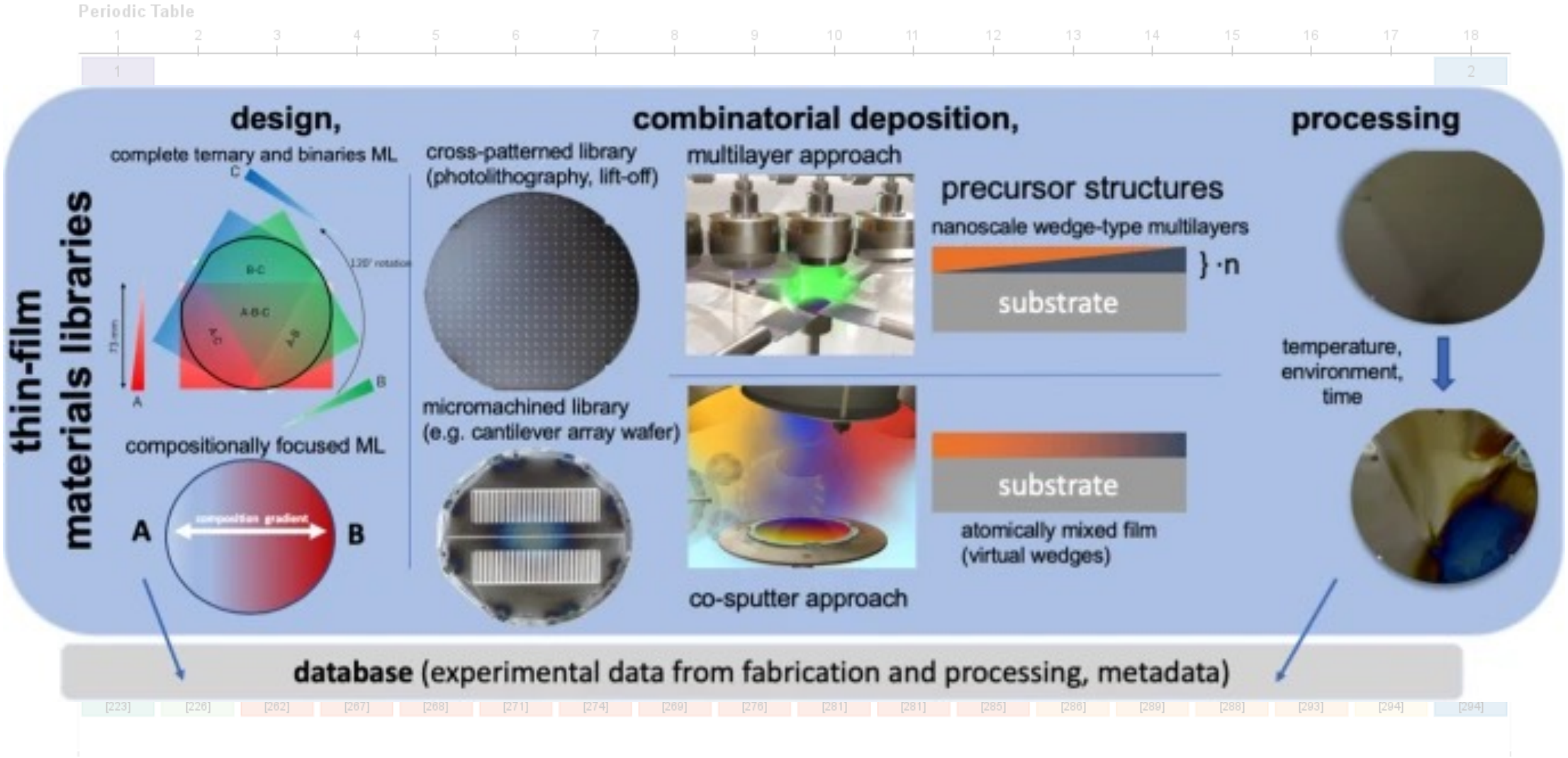
Challenge: Iterate over NIST potential database



L.F. Zhu, J. Janssen, et al. Comp. Mat. Sci. 187 (2021)

Combinatorial Synthesis Using Automated Labs

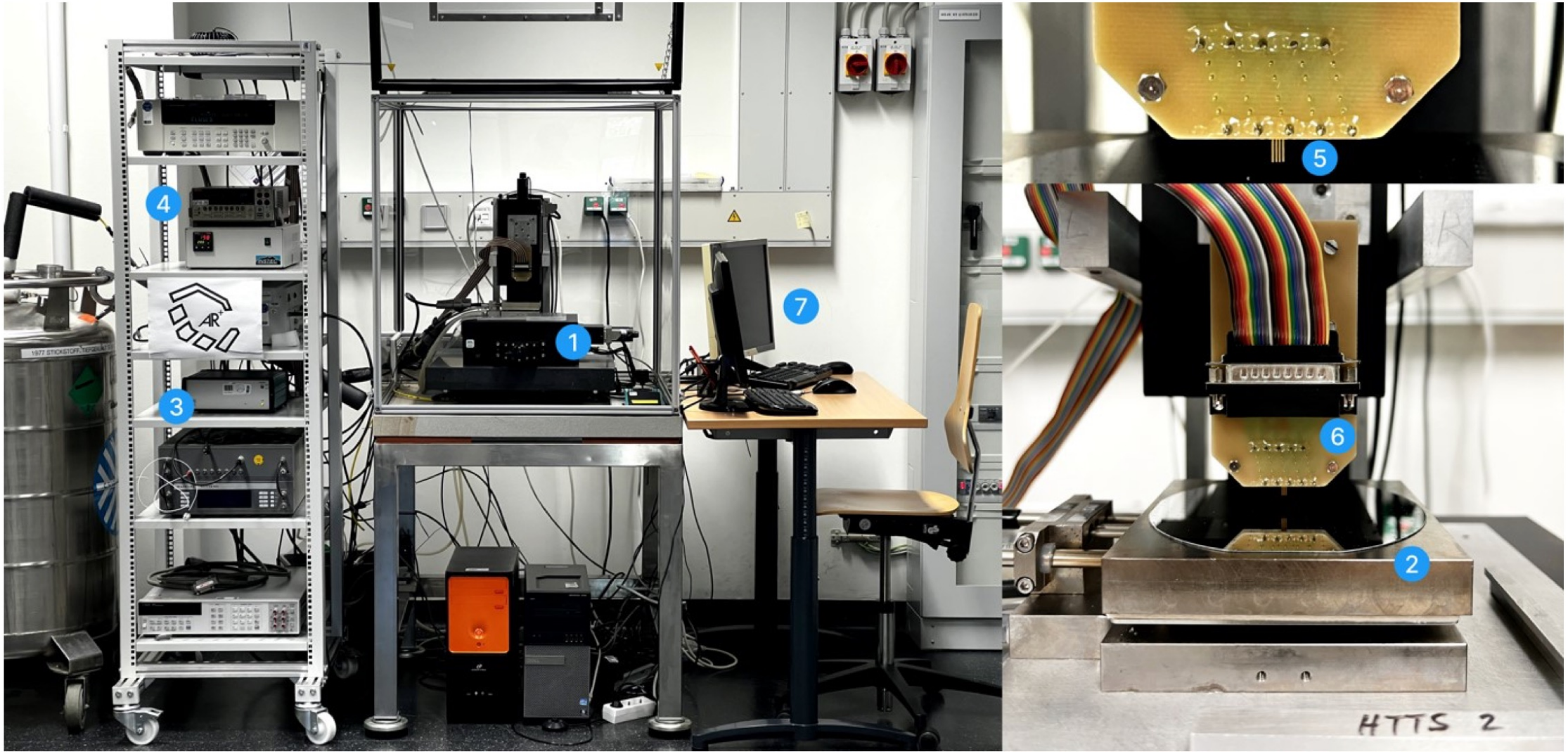
Iterate over the periodic table using composition-spread Materials Libraries



A. Ludwig, npj Computational Materials 5, 70 (2019).

Challenge: Measure Material Properties

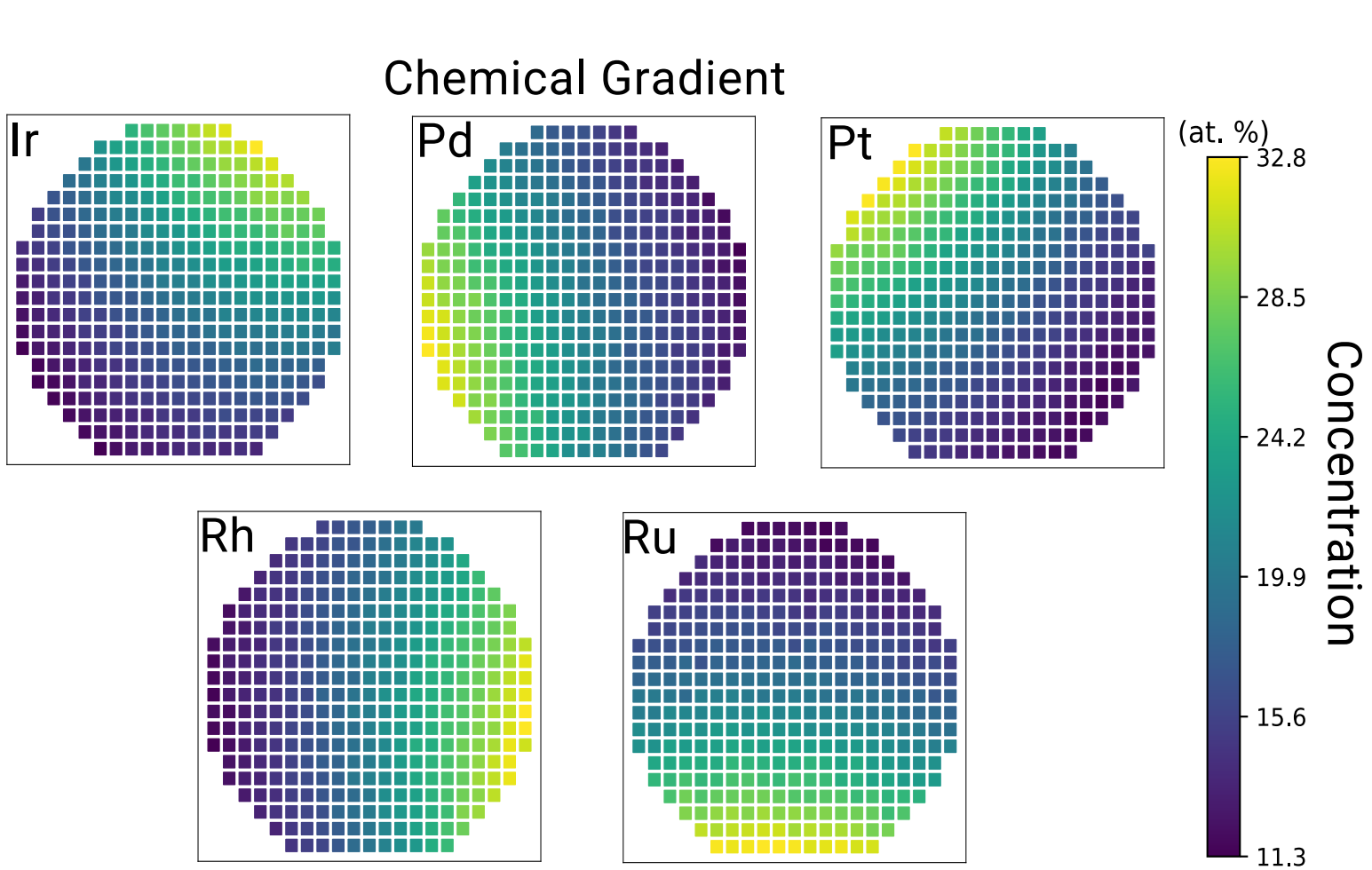
Mapped on 2D Hyperplane

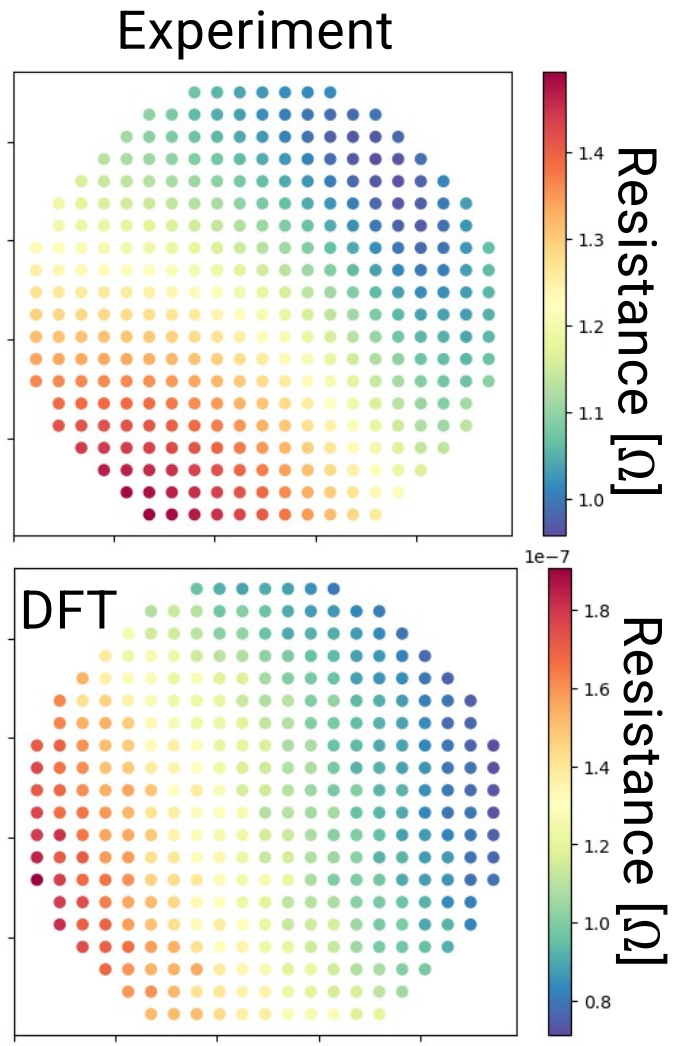


F. Thelen, L. Banko, R. Zehl, S. Baha, A. Ludwig. Digital Discovery, 2, 1612-1619 (2023)

Gaussian Process to Predict Resistivity

Couple Experiments and Density Functional Theory





M. Stricker, L. Banko, N. Sarazin, N. Siemer, J. Janssen, L. Zhang, J. Neugebauer, A. Ludwig, npj Comput. Mater., 12, 2 (2026).

Gaussian Process to Predict Resistivity

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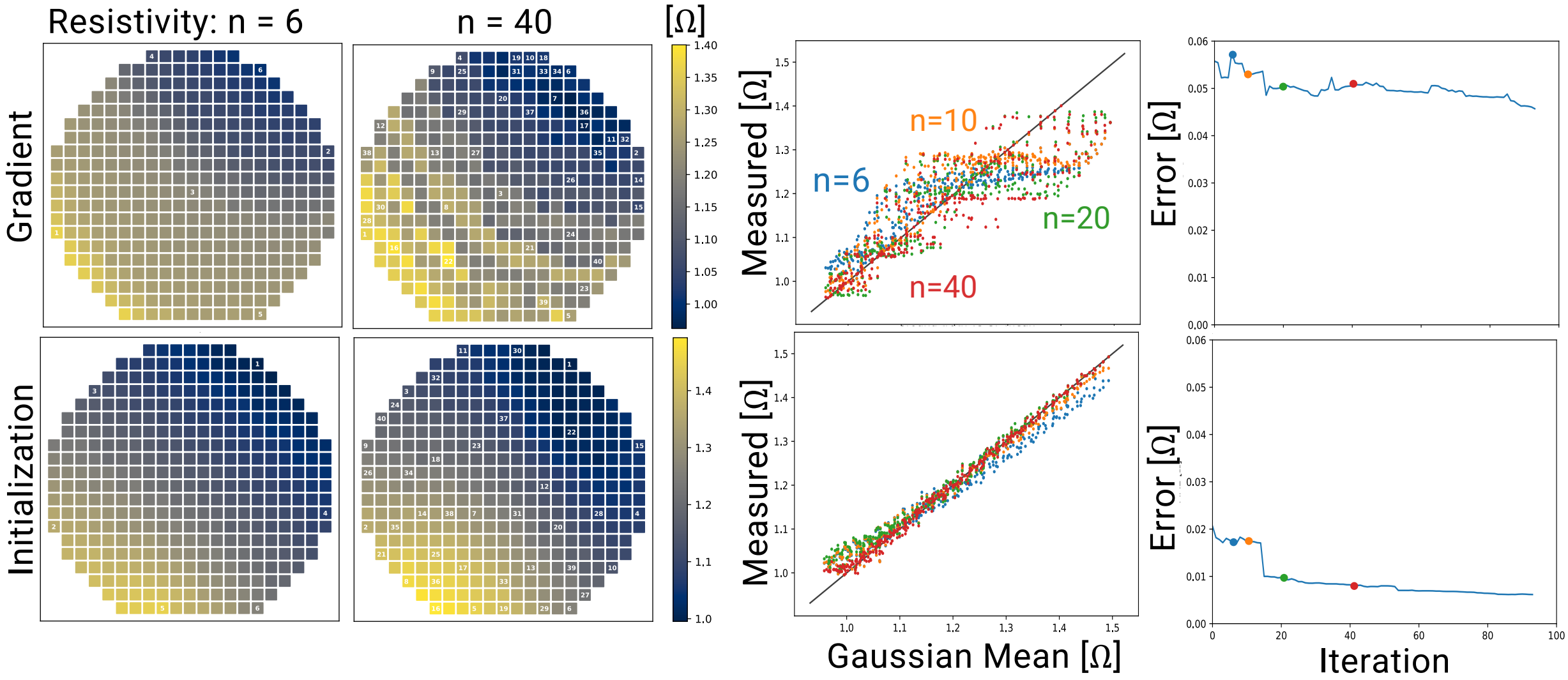
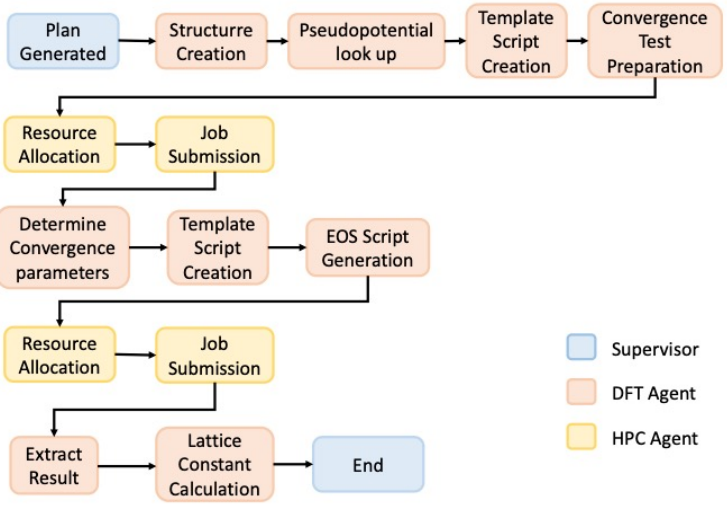


M. Stricker, L. Banko, N. Sarazin, N. Siemer, J. Janssen, L. Zhang, J. Neugebauer, A. Ludwig, npj Comput. Mater., 12, 2 (2026).

Workflows to Accelerate Materials Discovery – Thank you

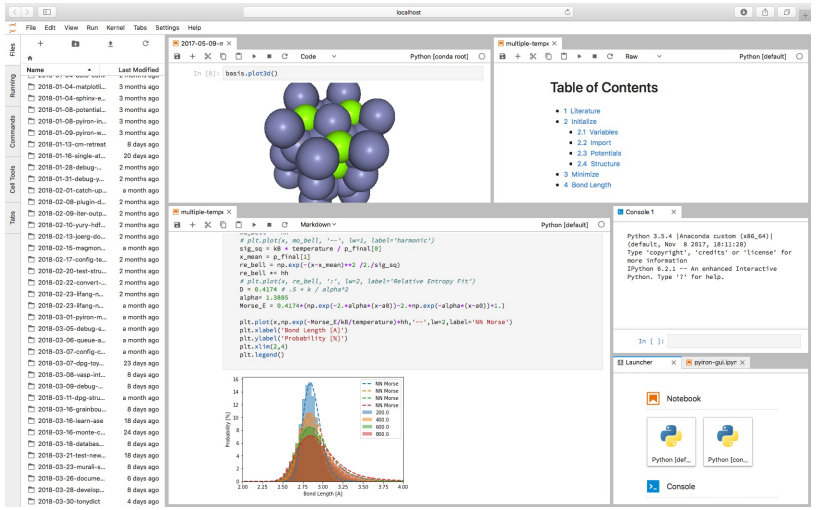
Artificial Intelligence bridges the gap between simulation and experiment

Large Language Model (LLM) Agents based on Functions



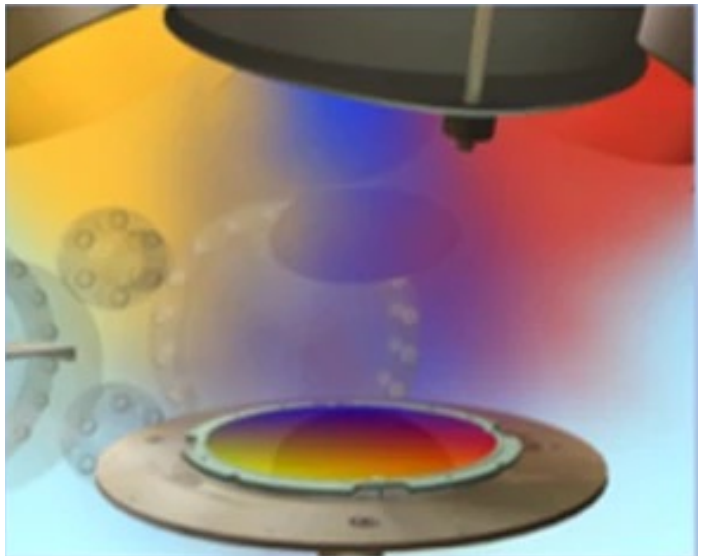
LLM agents provide LLMs with access to atomistic simulation and prevents the hallucination of LLMs.

pyiron Workflow Framework



The pyiron workflow framework provides a programmatic interface to simulation codes and high-performance computing.

Experimental Measurements are just another Python function



Materials Acceleration Platforms (MAP) combine simulation and experiment in the same workflow.