



# **OptiMat Alloys: a FAIR, living database of multi-principal element alloys enabled by a conversational agent**

**Yang Hu, Vladyslav Turlo**

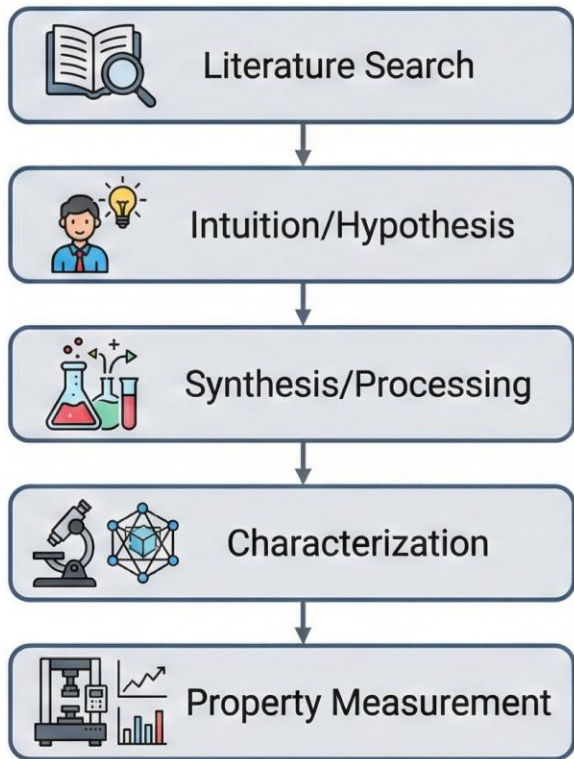
Laboratory for Advanced Materials  
Processing, Empa, Thun, Switzerland

22.09.2026

# Traditional materials discovery is slow



## Traditional materials discovery workflow



## Limitations



Process is slow



Labor-intensive



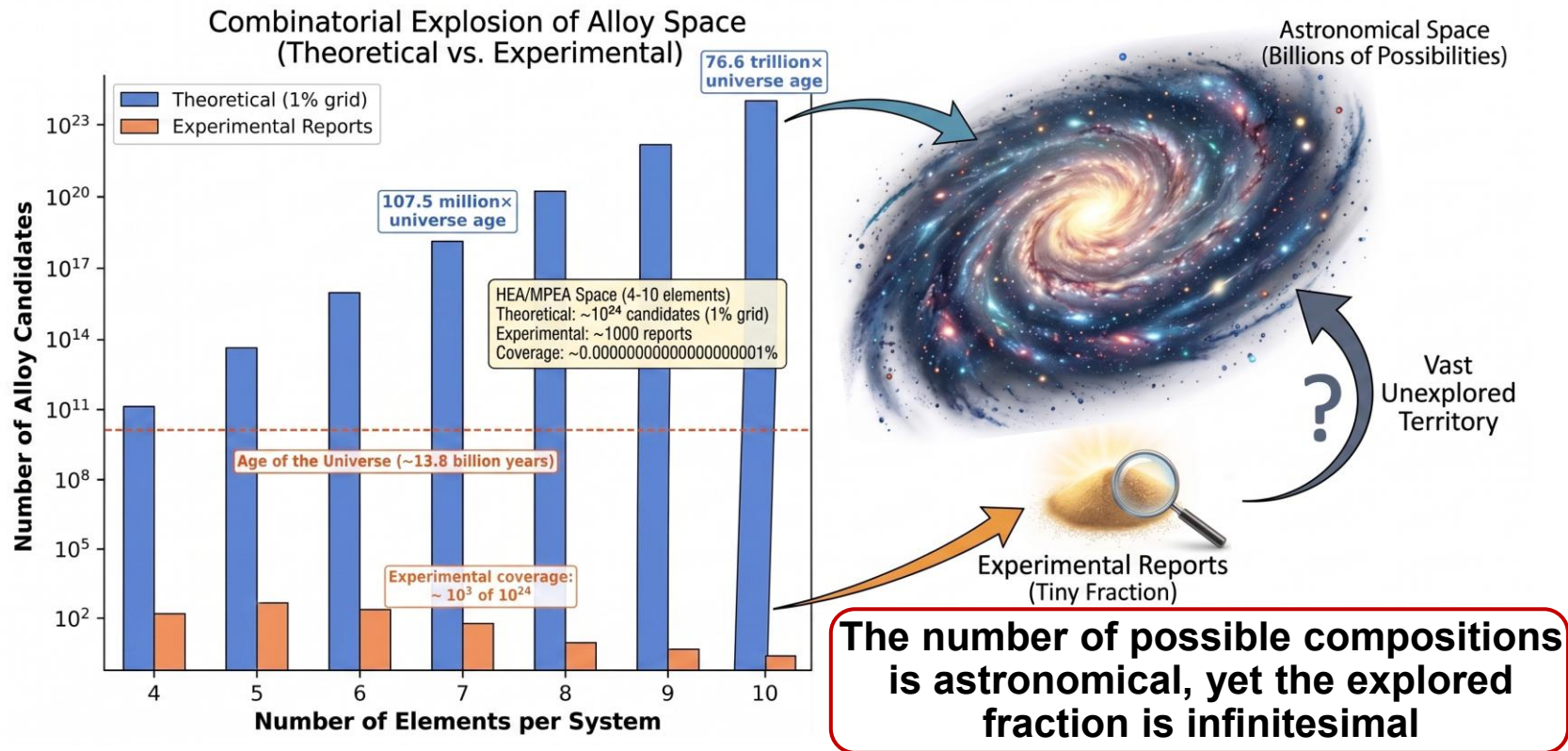
Linear & Sequential



Relies on "Edisonian" trial-and-error

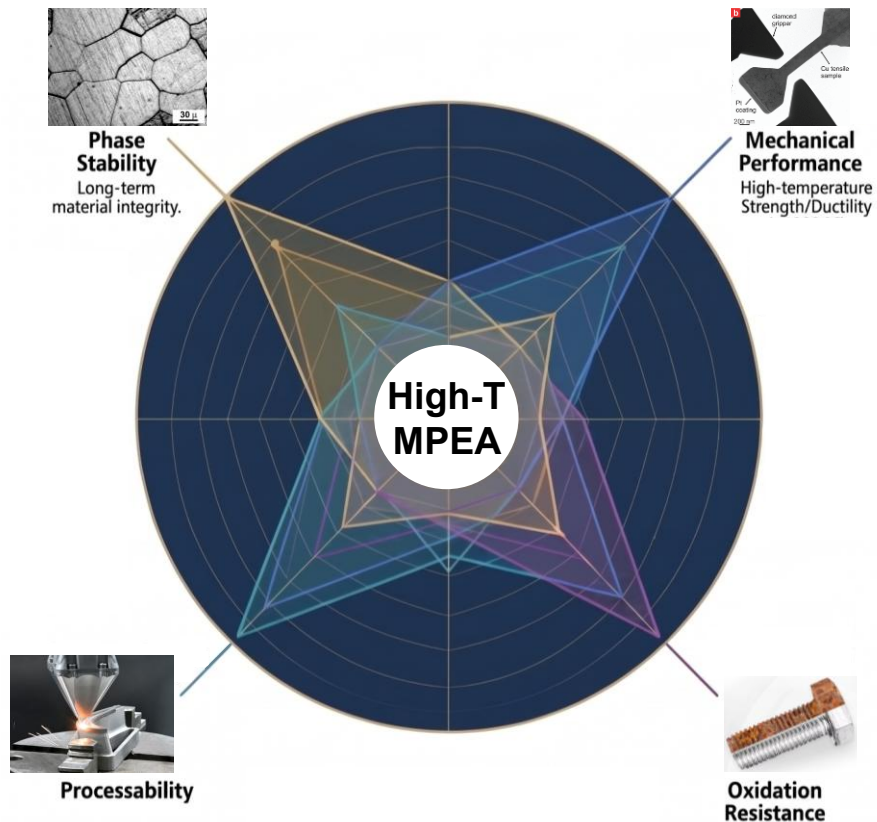
**High cost, long development cycles,  
low success rate**

# The design space of complex materials is vast



MPEA: multi-principal element alloy

# The design of complex materials is multi-objective



## Space propulsion



## Gas turbine



## Fusion and fission applications



Potential applications

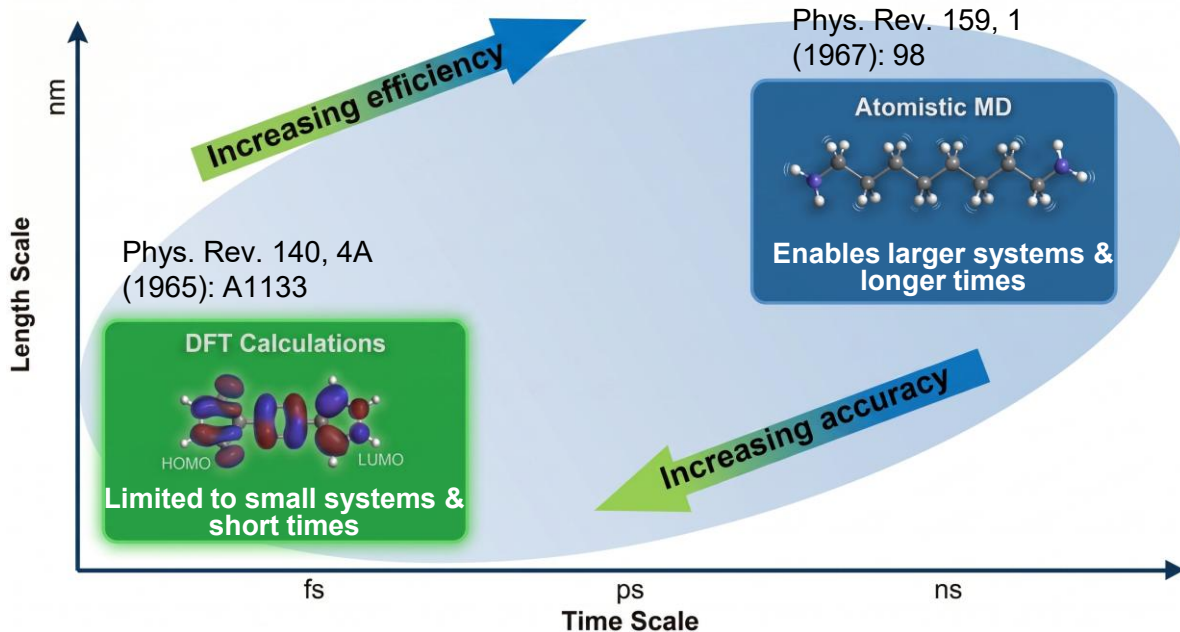
# Simulations can accelerate materials discovery



## Robust Atomistic Codes



Mature simulation engines provide a reliable foundation for executing complex workflows.

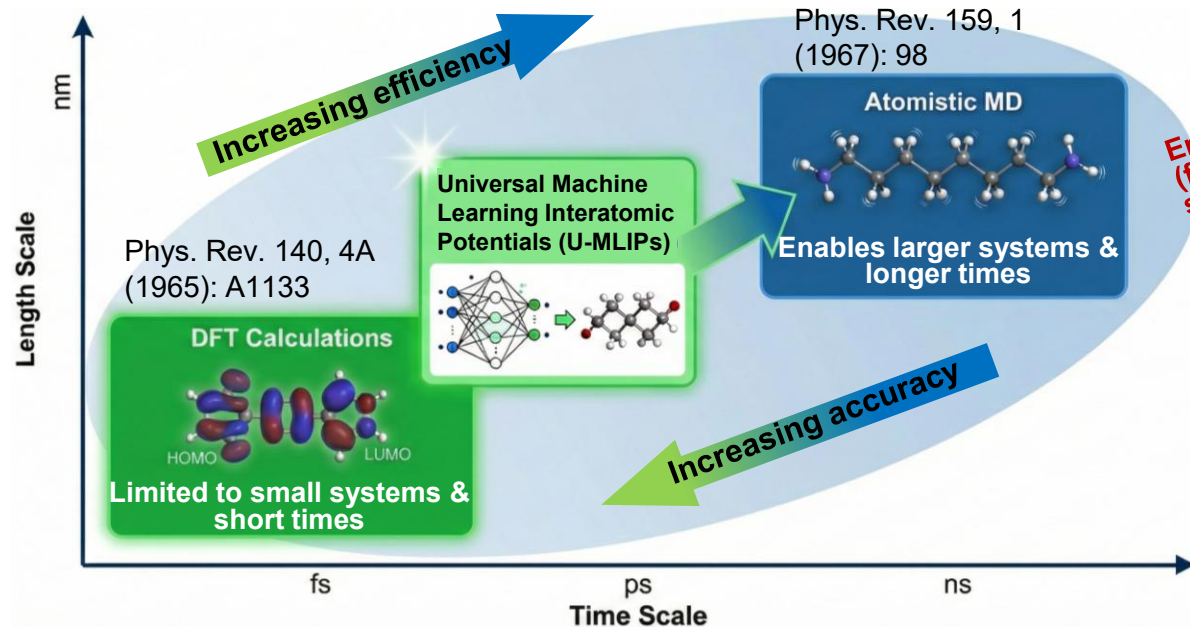


J. Comput. Phys. 117, 1 (1995): 1-19

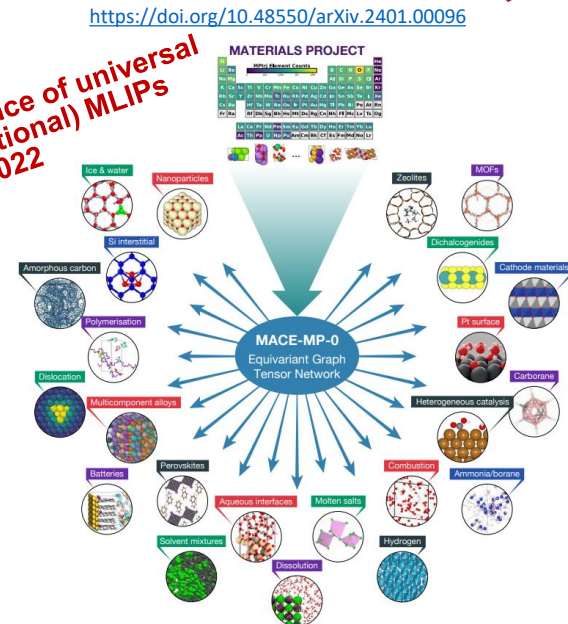
Phys. Rev. B 54, 16 (1996): 11169

J. Phys. Condens. Matter 29, 27 (2017): 273002

# U-MLIPs expand atomistic simulation capabilities



**Emergence of universal (foundational) MLIPs since 2022**



**Breakthroughs enabled by U-MLIPs:**

- Near-DFT accuracy
- Broad elemental coverage
- Scalable simulations

# U-MLIPs expand atomistic simulation capabilities



## Accuracy of U-MLIPs:

| Calculator    | Training data          | Formation energy<br>MAE (meV/atom) | R <sup>2</sup> | Stability<br>F1 score |
|---------------|------------------------|------------------------------------|----------------|-----------------------|
| NequIP oam-xl | OMat24 + MPtrj + sAlex | 19.5                               | 0.995          | 0.885                 |
| ORB v3 (mpa)  | MPtrj + Alex + OMat24  | 22.7                               | 0.993          | 0.887                 |
| MACE mpa-0    | MPtrj + sAlex          | 27.6                               | 0.994          | 0.836                 |

Nat. Mach. Intell. 7, no. 6 (2025), 836-847.

npj Comput. Mater. 7, no. 1 (2021): 12.

## Computational efficiency of U-MLIPs:

| Supercell | Atoms | VASP<br>GPU | U-MLIP wall-clock time per forward pass (ms) |                    |                |                  | Speedup                |
|-----------|-------|-------------|----------------------------------------------|--------------------|----------------|------------------|------------------------|
|           |       |             | ORB v3<br>direct                             | ORB v3<br>conserv. | MACE<br>omat-0 | NequIP<br>oam-xl |                        |
| 2×2×2     | 32    | 11.6 min    | 11                                           | 28                 | 27             | 183              | ~6.3×10 <sup>4</sup> x |
| 3×3×3     | 108   | 79.5 min    | 12                                           | 78                 | 59             | 766              | ~3.8×10 <sup>5</sup> x |
| 4×4×4     | 256   | 3.78 days   | 16                                           | 184                | 122            | 2,215            | ~2.0×10 <sup>7</sup> x |

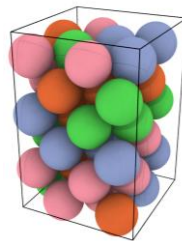


## Matbench Discovery

[matbench-discovery.materialsproject.org](https://matbench-discovery.materialsproject.org)

- Community benchmark for U-MLIPs
- Test set — WBM (Wang–Botti–Marques):  
256,963 inorganic crystals covering 85 elements.  
42% are intermetallics; the rest are oxides, halides, chalcogenides, pnictides and borides/carbides. 16.7% lie on the DFT convex hull, i.e. are stable.

Ni Fe Co Cr



- Laptop GPU: RTX 5000 Ada, 16 GB
- VASP: single-point calculation
- U-MLIPs: one forward pass (energy+forces)
- Speedup = VASP / ORB direct

# Simulations can accelerate materials discovery



## Robust Atomistic Codes



Mature simulation engines provide a reliable foundation for executing complex workflows.

## Universal ML Potentials



**UPET**  
UNIVERSAL ATOMISTIC MODELS

Pre-trained foundation models offer near-DFT accuracy across broad compositions without system-specific fitting.



**Simulations are powerful, but the barrier to entry is high and progress is limited by manual setup, monitoring, and analysis.**

**How can we make simulations more accessible?**

**How can we free researchers from routine, repetitive tasks?**

arXiv:2410.22570 (2024) Nat. Commun. 16, 1 (2025): 10653

arXiv:2607.28461 (2026) J. Chem. Phys. 163, 18 (2025)

# Agentic materials discovery is now possible!



## Robust Atomistic Codes



## Universal ML Potentials



UPET  
UNIVERSAL ATOMIC MODELS

## Reasoning-Capable LLMs



ChatGPT



MIMO



An **agent** is a software system that can **plan and take actions** toward a goal. In practice, it is an orchestrator that connects tools, data, and decision-making logic.

arXiv:2303.08774 (2023)

arXiv:2406.12793 (2024)

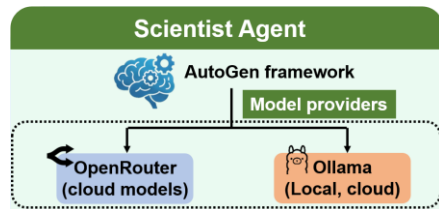
arXiv:2505.07608

(2025)

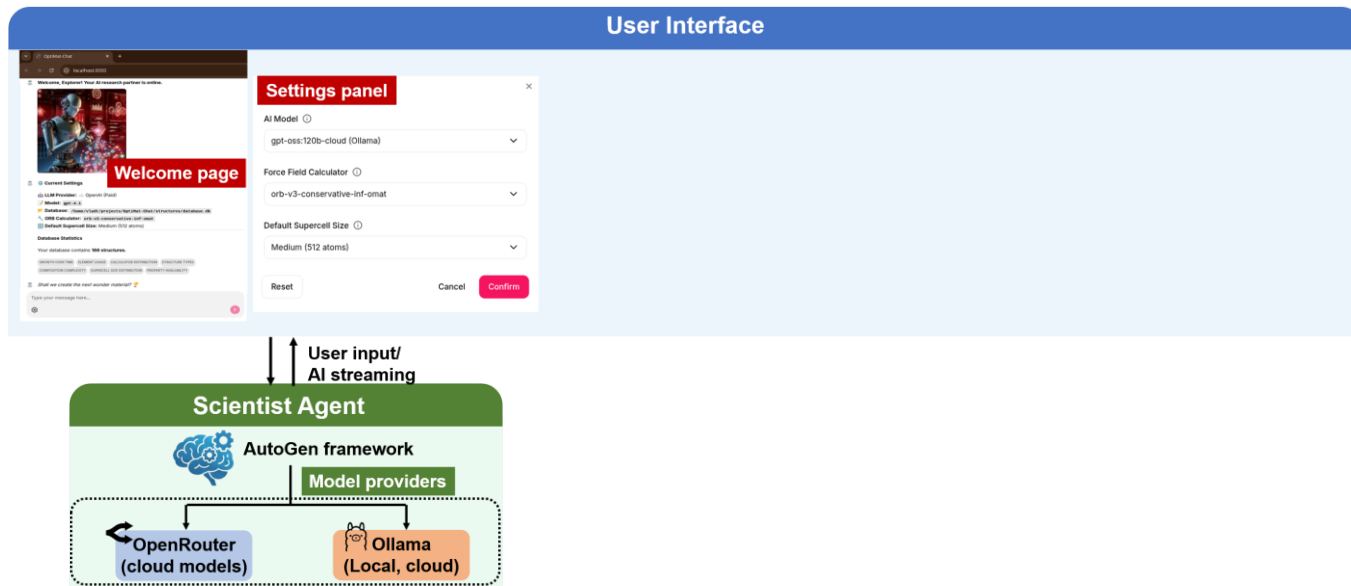
# OptiMat Alloys architecture



- OptiMat Alloys is built on the Python-based **AutoGen** framework.
- AutoGen is an open-source framework developed by Microsoft for building multi-agent AI applications.
- The agent connects to cloud-hosted LLMs via APIs.



# OptiMat Alloys architecture



- The agent provides a web-based GUI built with Chainlit.
- Users interact with it entirely in natural language.

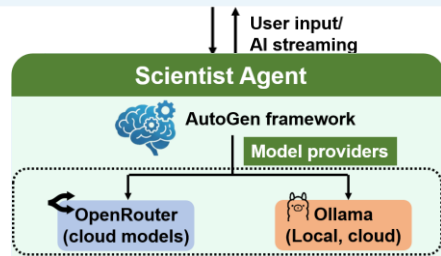
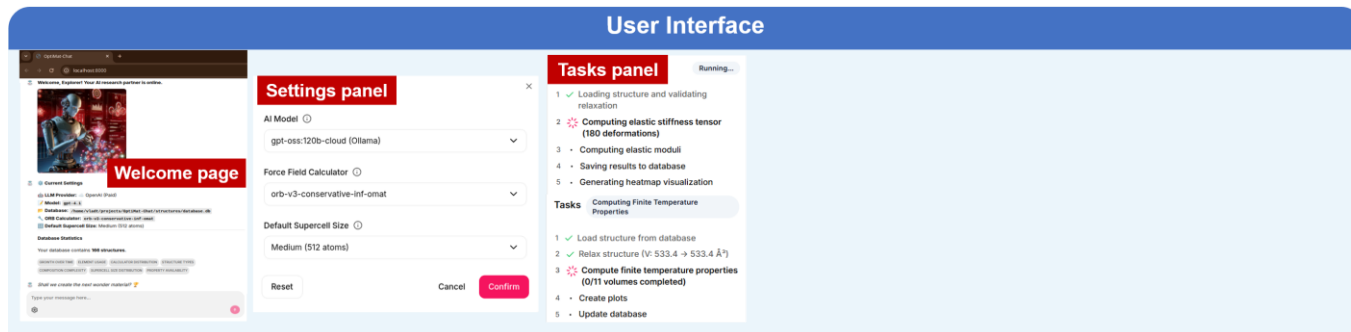
# OptiMat Alloys architecture



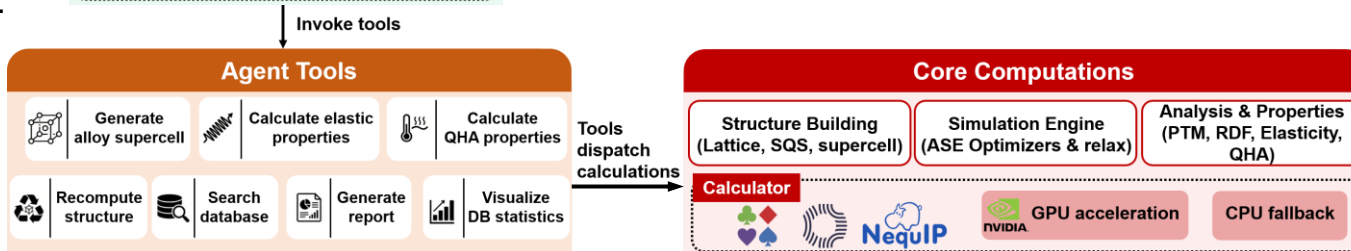
## ASE:

a Python toolkit for setting up, running, and analyzing atomistic simulations.

**U-MLIPs** are installed as Python packages and used as calculators within ASE.



➤ The agent integrates ASE-based simulation tools with embedded visualization via OVITO and Plotly.

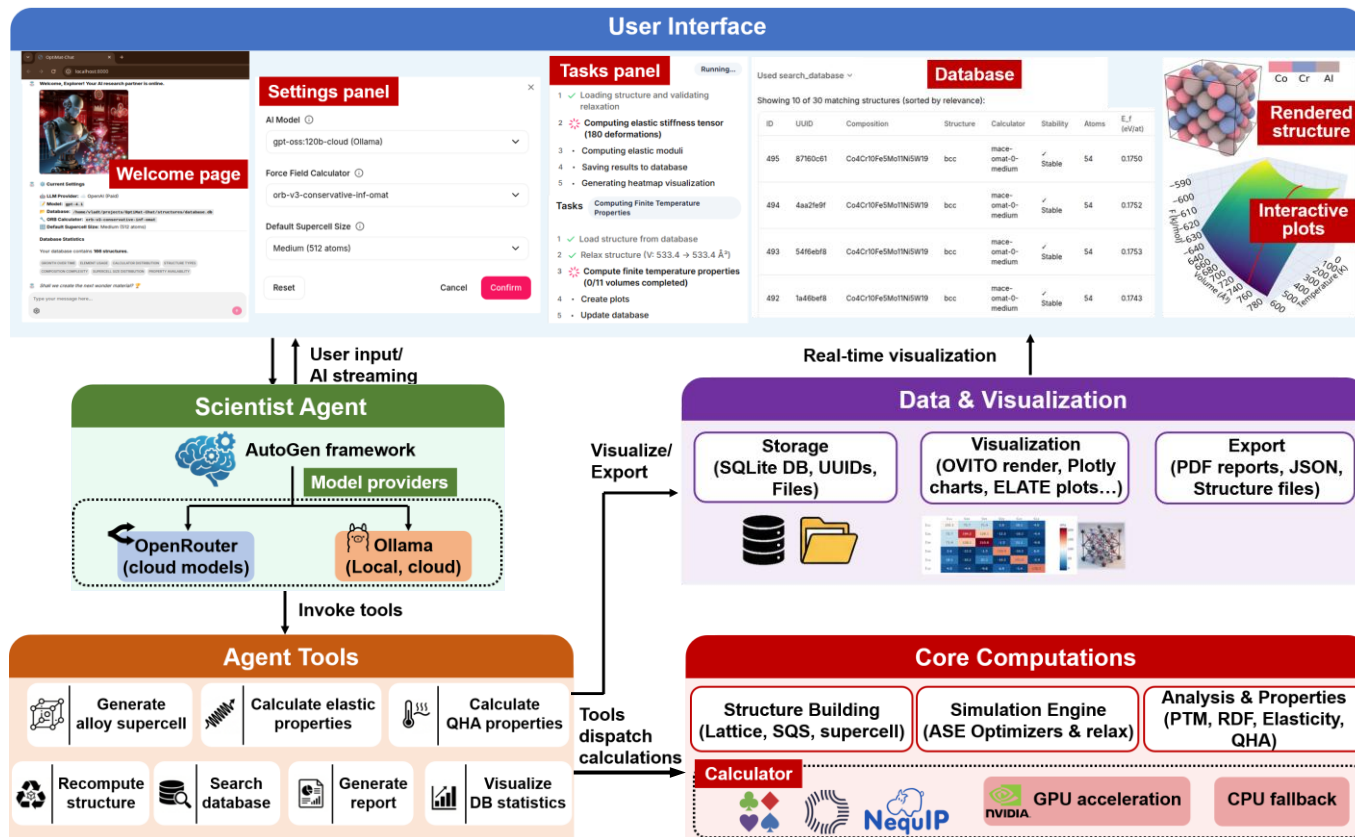


# OptiMat Alloys architecture

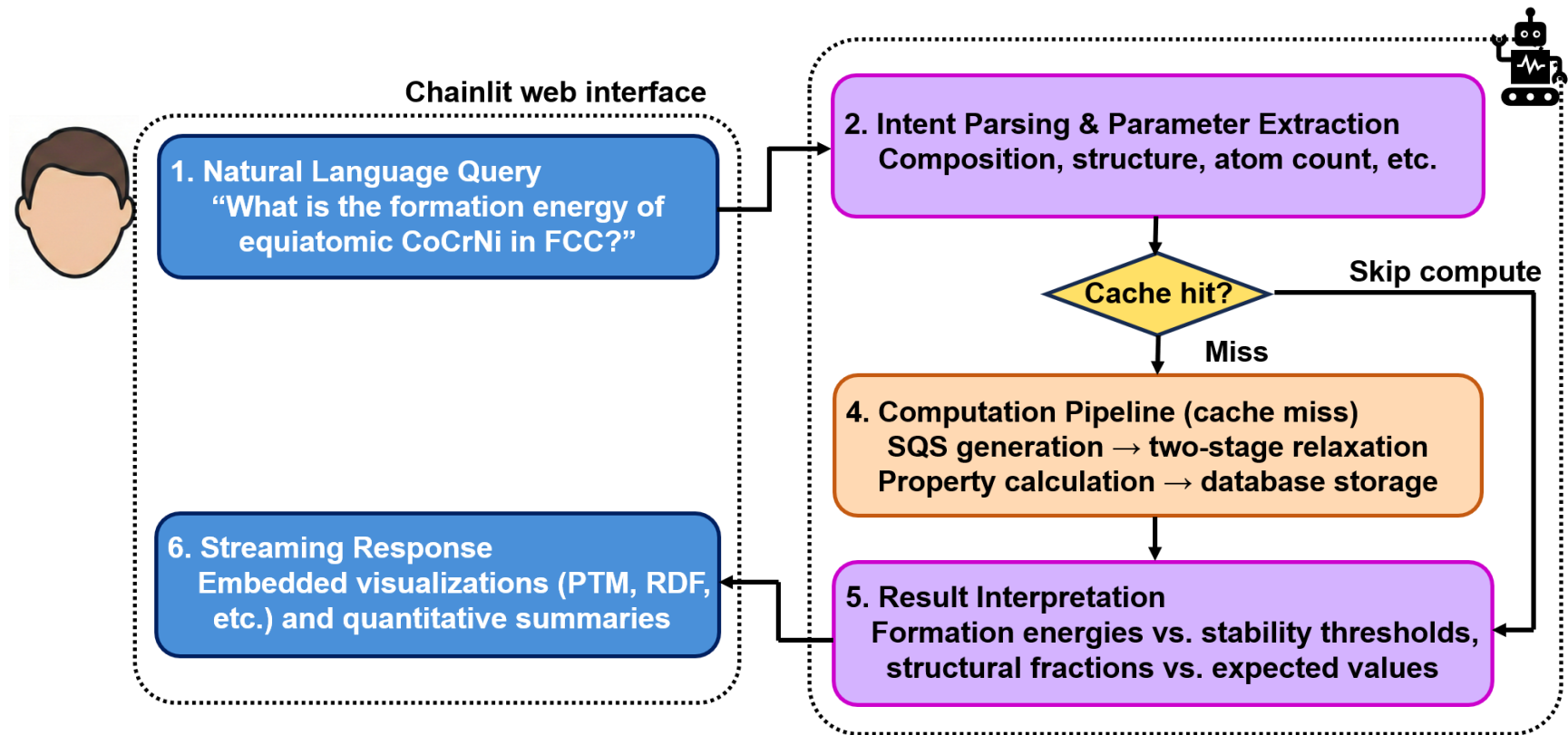


➤ The agent writes computed data into a local SQLite database.

➤ Simulation inputs and results can be summarized and exported as a report.



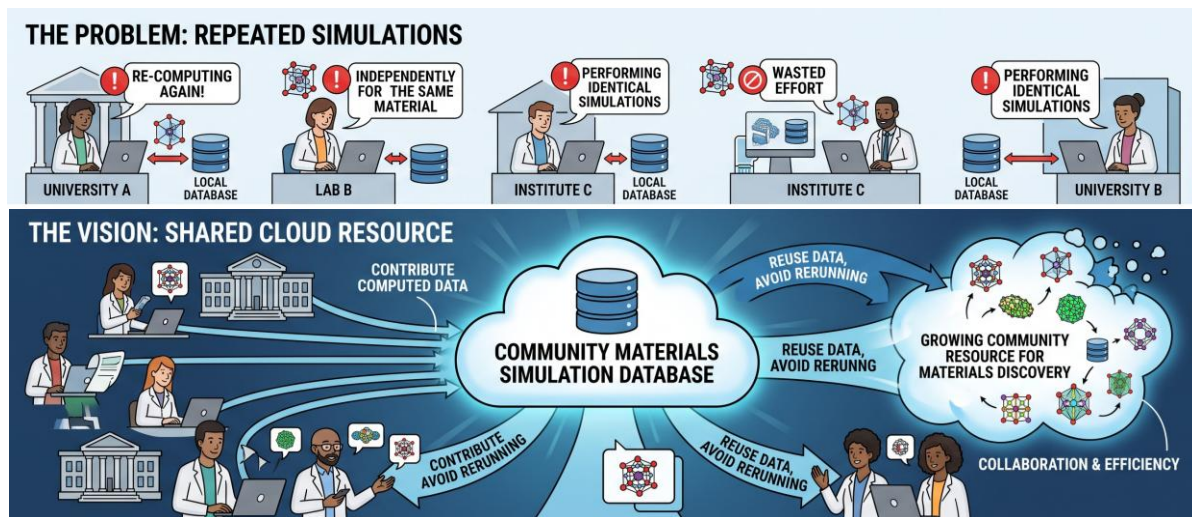
# Agent decision and execution flow



# A living database that grows through usage



- The local SQLite database grows with every user-agent interaction.
- Data generation is no longer separated from data deposition
- Stored results avoid repeated computation



# Beyond results: capturing simulation provenance



- Simulation methods, input parameters, and software versions are summarized in an exportable report.
- Generated structures can also be exported for external use.

## Single Crystal Elastic Properties

**Directional Properties:** Single crystal elastic properties vary with crystallographic direction due to anisotropy. All directional properties are computed from the compliance tensor  $S = C^{-1}$ :

**Young's modulus:**  $1/E(n) = S_{ijkl} n_i n_j n_k n_l$ . **Linear compressibility:**  $\beta(n) = S_{ijkl} \delta_{ki} n_j n_l$ . **Shear modulus:**  $1/G(n,m) = 4 S_{ijkl} n_i m_j n_k m_l$ . **Poisson's ratio:**  $\nu(n,m) = -S_{ijkl} n_i n_j m_k m_l / S_{ijkl} n_i n_j n_k n_l$ , where  $S_{ijkl}$  is the compliance tensor,  $\delta_{ki}$  is the Kronecker delta,  $n$  is the loading direction, and  $m$  is the perpendicular direction for lateral response.

**Auxetic Behavior:** Negative Poisson's ratio in certain directions indicates the material expands laterally when stretched (unusual mechanical behavior).

**Wave velocities:**  $v_s(n) = \sqrt{G(n)/\rho}$  for shear waves,  $v_l(n) = \sqrt{((K(n) + 4G(n)/3)/\rho)}$  for longitudinal/compression waves, where  $v_s$  is the shear wave velocity,  $v_l$  is the longitudinal wave velocity,  $G(n)$  is the directional shear modulus,  $K(n)$  is the directional bulk modulus,  $n$  is the propagation direction, and  $\rho$  is the material density.

| Property                           | Min     | Max    | Unit  |
|------------------------------------|---------|--------|-------|
| Young's Modulus (E)                | 128.74  | 331.65 | GPa   |
| Shear Modulus (G)                  | 46.26   | 139.97 | GPa   |
| Poisson's Ratio ( $\nu$ )          | -0.1395 | 0.6964 |       |
| Linear Compressibility ( $\beta$ ) | 1.822   | 2.053  | 1/TPa |

## Software Versions

ASE: 3.26.0, Phonopy: 2.43.6, OVITO: 3.11.1, PyTorch: 1.8.0+cu128, NumPy: 2.3.4, ORB Models: v0.5.5, MACE: 0.3.14, NequIP: 0.16.1, phono3py: 3.19.4, sqsgenerator: (0, 5, 3), MechElastic: 1.2.29

## 4. Computational Methods

### NequIP Equivariant Neural Network Potential

E(3)-equivariant neural network potential with state-of-the-art accuracy. OAM models trained on OMat24, MPtrj, and sAlex datasets (112.8M structures). MP models trained on MPtrj only (1.58M structures). [7, 8]

| Parameter    | Value                                                   |
|--------------|---------------------------------------------------------|
| Model used   | nequip-oam-l                                            |
| Model Oam L  | nequip-oam-l (~15M params, F1=0.893)                    |
| Model Oam XI | nequip-oam-xi (~15M params, F1=0.906, highest accuracy) |
| Model Mp L   | nequip-mp-l (9.6M params, MPtrj only)                   |
| Precision    | float32                                                 |

### Special Quasirandom Structure (SQS)

Generates special quasirandom structures that best approximate the correlation functions of a random alloy. Minimizes short-range order to represent disordered solid solutions. [9, 10]

| Parameter     | Value                                                                    |
|---------------|--------------------------------------------------------------------------|
| Method        | sqsgenerator (0, 5, 3)                                                   |
| Target        | Minimize pair correlation deviation                                      |
| Iterations    | 1,000,000 Monte Carlo steps (vol default; library default is 10,000,000) |
| Shell Weights | (1: 1.0, 2: 0.5) — Monte Carlo, 2nd NN half-weighted                     |

|                  |             |
|------------------|-------------|
| POSCAR           | File        |
| structure.cif    | CIF File    |
| structure.lammps | LAMMPS File |
| structure.xyz    | XYZ File    |



Opti**Mat**  
.Chat

Materials Discovery Through Conversation

Veo

# Take-home messages



- **Agentic materials discovery is possible today.** Robust atomistic codes, universal ML potentials and reasoning-capable LLMs are all mature; the agent is the glue.
- **U-MLIPs bring near-DFT accuracy at a tiny fraction of the cost.** Formation energies within 30 meV/atom of DFT on Matbench Discovery; cost scales roughly linearly with system size, against  $N^3$  for DFT.
- **OptiMat Alloys turns a sentence into simulations.** SQS structures, elastic tensors and finite-temperature thermodynamics, with no scripts, no job files and no HPC account.
- **Every result persists with its provenance.** A FAIR living database that grows through use (491 structures in six months of testing) and can be merged across groups.
- **Screening-grade, not final.** Promising compositions still need DFT and experiment; the calculator is swappable as better potentials arrive.

# Empa – The Place where Innovation Starts



<https://www.optimat.chat/>

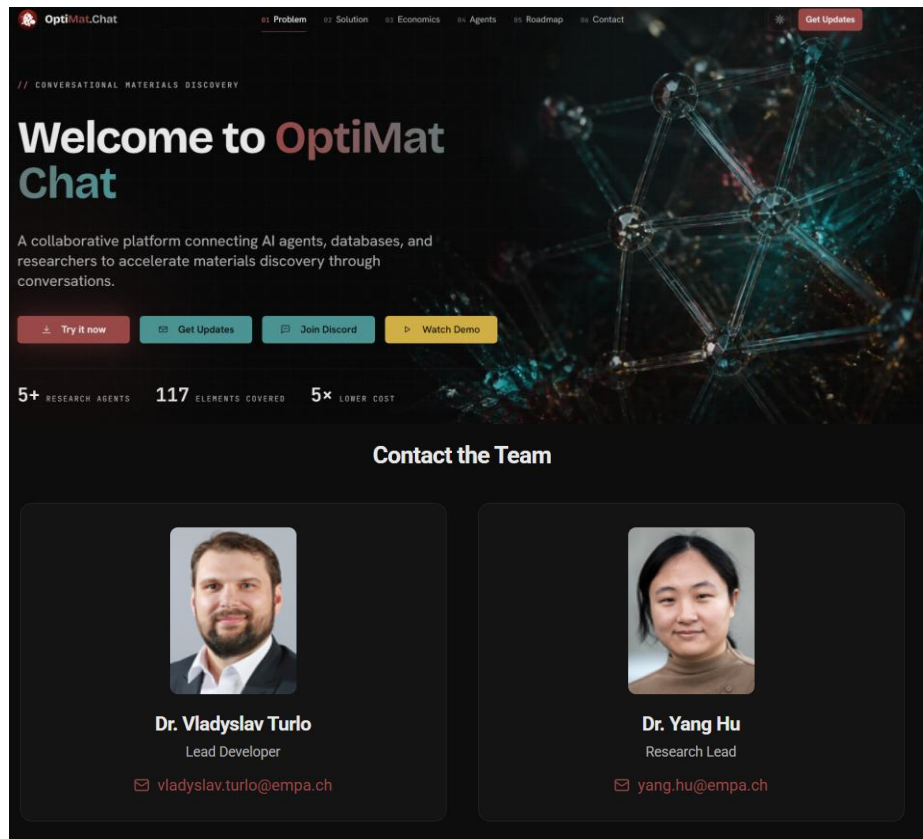
<https://github.com/OptiMat-Chat/OptiMat-Alloys>

Docker image: [yhu1991/optimat-alloys](#)

[yang.hu@empa.ch](mailto:yang.hu@empa.ch)



## Thank you!



# Accuracy of U-MLIPs



Mean Absolute Error of predicted vs.  
DFT convex hull distance (lower=better)

Full Test Set

Unique Prototypes

| #  | Model                 | CPS ↑ | Acc   | F1    | DAF   | Prec  | MAE   | R <sup>2</sup> | K <sub>SRME</sub> | RMSD  | CMD5  | CDS   | Params | Targets            | Date Added | Links                                                                                                       | r <sub>cut</sub> | Training Set                   | Org |
|----|-----------------------|-------|-------|-------|-------|-------|-------|----------------|-------------------|-------|-------|-------|--------|--------------------|------------|-------------------------------------------------------------------------------------------------------------|------------------|--------------------------------|-----|
| 1  | TECE-OAM-RRR-1.0      | 0.908 | 0.978 | 0.929 | 6.073 | 0.928 | 0.018 | 0.871          | 0.093             | 0.058 | 0.630 | 0.270 | 222M   | EFS <sub>G</sub>   | 2026-07-05 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 2  | EquiFlashV2           | 0.907 | 0.978 | 0.929 | 6.069 | 0.928 | 0.018 | 0.873          | 0.094             | 0.058 | n/a   | n/a   | 44.9M  | EFS <sub>G</sub>   | 2026-06-11 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 3  | EquiformerV3+DeNS-OAM | 0.902 | 0.978 | 0.931 | 6.074 | 0.928 | 0.018 | 0.868          | 0.118             | 0.059 | n/a   | n/a   | 30.3M  | EFS <sub>G</sub>   | 2026-04-07 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 4  | GRACE-3L-OAM-L        | 0.900 | 0.977 | 0.925 | 6.041 | 0.923 | 0.018 | 0.875          | 0.121             | 0.058 | 0.739 | 0.699 | 42.1M  | EFS <sub>G</sub>   | 2026-07-02 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 5  | PET-OAM-XL            | 0.898 | 0.977 | 0.924 | 6.075 | 0.929 | 0.019 | 0.864          | 0.119             | 0.060 | 0.634 | 0.388 | 730M   | EFS <sub>G</sub>   | 2026-01-10 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | n/a              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 6  | TACE-OAM-L            | 0.889 | 0.972 | 0.910 | 5.898 | 0.902 | 0.020 | 0.868          | 0.126             | 0.061 | 0.728 | 0.761 | 82.9M  | EFS <sub>G</sub>   | 2026-04-09 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 7  | eSEN-30M-OAM          | 0.888 | 0.977 | 0.925 | 6.069 | 0.928 | 0.018 | 0.866          | 0.17              | 0.061 | 0.625 | 0.648 | 30.2M  | EFS <sub>G</sub>   | 2025-03-17 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 8  | EquiFlash             | 0.888 | 0.975 | 0.919 | 5.983 | 0.915 | 0.019 | 0.871          | 0.158             | 0.060 | n/a   | n/a   | 28.7M  | EFS <sub>G</sub>   | 2025-06-23 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 9  | Nequip-OAM-XL         | 0.886 | 0.971 | 0.906 | 5.869 | 0.897 | 0.020 | 0.872          | 0.125             | 0.063 | 0.623 | 0.796 | 32.1M  | EFS <sub>G</sub>   | 2025-11-30 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 10 | MatRIS-10M-OAM        | 0.877 | 0.976 | 0.921 | 6.039 | 0.923 | 0.019 | 0.871          | 0.218             | 0.060 | 0.581 | 0.678 | 10.4M  | EFS <sub>G</sub> M | 2025-10-29 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 11 | SevenNet-Omni-i12*    | 0.873 | 0.971 | 0.906 | 5.954 | 0.910 | 0.021 | 0.868          | 0.192             | 0.062 | 0.626 | 0.696 | 54.9M  | EFS <sub>G</sub>   | 2026-01-12 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 243M COSMOSDataset             |     |
| 12 | Nequip-OAM-L          | 0.870 | 0.967 | 0.893 | 5.823 | 0.890 | 0.022 | 0.865          | 0.166             | 0.065 | 0.670 | 0.818 | 9.6M   | EFS <sub>G</sub>   | 2025-09-08 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 13 | GRACE-2L-OAM-L        | 0.865 | 0.964 | 0.883 | 5.840 | 0.893 | 0.022 | 0.862          | 0.169             | 0.064 | 0.759 | 0.694 | 26.4M  | EFS <sub>G</sub>   | 2025-09-09 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 14 | ORB v3                | 0.860 | 0.971 | 0.905 | 5.912 | 0.904 | 0.024 | 0.821          | 0.21              | 0.075 | n/a   | n/a   | 25.5M  | EFS <sub>G</sub>   | 2025-04-05 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 6.47M (133M) MPtrj+Alex+OMat24 |     |
| 15 | DPA-4.0.1-Pro-MPtrj   | 0.840 | 0.956 | 0.857 | 5.609 | 0.857 | 0.029 | 0.836          | 0.211             | 0.069 | 0.598 | n/a   | 22.8M  | EFS <sub>G</sub>   | 2026-06-11 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 146k (1.58M) MPtrj             |     |
| 16 | Allegro-OAM-L         | 0.840 | 0.966 | 0.895 | 5.674 | 0.867 | 0.022 | 0.868          | 0.319             | 0.065 | 0.602 | 0.828 | 9.7M   | EFS <sub>G</sub>   | 2025-09-08 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 7 Å              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 17 | GRACE-2L-OAM          | 0.837 | 0.963 | 0.880 | 5.774 | 0.883 | 0.023 | 0.862          | 0.294             | 0.067 | 0.751 | 0.527 | 12.6M  | EFS <sub>G</sub>   | 2025-02-06 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 6.6M (113M) MPtrj+OMat24+sAlex |     |
| 18 | EquiformerV3+DeNS-MP  | 0.830 | 0.956 | 0.863 | 5.479 | 0.838 | 0.029 | 0.840          | 0.275             | 0.070 | n/a   | n/a   | 30.3M  | EFS <sub>G</sub>   | 2026-04-07 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 146k (1.58M) MPtrj             |     |
| 19 | DPA-3.1-3M-FT         | 0.802 | 0.963 | 0.884 | 5.667 | 0.866 | 0.023 | 0.869          | 0.469             | 0.069 | 0.647 | 0.533 | 3.27M  | EFS <sub>G</sub>   | 2025-06-05 | <a href="#">🔗</a> <a href="#">📄</a> <a href="#">📊</a> <a href="#">📈</a> <a href="#">📉</a> <a href="#">📊</a> | 6 Å              | 163M OpenLAM                   |     |

Acc: Accuracy of classifying crystals as thermodynamically stable or unstable (higher=better)

F1 Score: Harmonic mean of precision and recall for stable/unstable material classification (higher=better)

Prec: Precision of classifying thermodynamic stability (higher=better)

R<sup>2</sup>: Coefficient of determination (higher=better)



# Thermo-Calc and experimental databases

16 Thermo-Calc databases (TCFE14, TCHEA8, TCNI13, TCAL10, TCCU6, TCTI6, TCMG8, TCMO2, TCNB1, TCNOBL4, TCSI1, TCSLD5, TCZR1, TCCC1, TCPMAG2, TCUHTM2) as of October 2025

Table S1: Thermo-Calc thermodynamic database coverage across 67 metallic elements, filtered to exclude impurity-containing systems. Theoretical space is  $\binom{67}{n}$  for  $n$ -component systems.

| System order       | ThermoCalc   | Theoretical       | Coverage (%) |
|--------------------|--------------|-------------------|--------------|
| Binary             | 2,185        | 2,211             | 98.82        |
| Ternary            | 185          | 47,905            | 0.39         |
| Quaternary         | 7            | 766,480           | 0.0009       |
| Quinary            | 1            | 9,657,648         | 0.00001      |
| <b>Total (2–5)</b> | <b>2,378</b> | <b>10,474,244</b> | <b>0.02</b>  |

Table S2: Application-domain distribution of 1,089 unique experimental HEA/MPEA compositions. Compositions may appear in multiple domains; percentages are relative to total entries (2,004).

(i) the Borg MPEA Database hosted by Citrine Informatics (630 compositions), and (ii) 29 domain-specific review papers published between 2018 and 2024 (705 compositions, 459 unique after deduplication with the Borg set).

| Application domain           | Count | Percentage (%) |
|------------------------------|-------|----------------|
| Structural (BCC HEAs)        | 240   | 12.0           |
| Refractory HEAs              | 220   | 11.0           |
| Biomedical                   | 215   | 10.7           |
| Computational                | 209   | 10.4           |
| Refractory (processing)      | 192   | 9.6            |
| Nuclear / irradiation        | 180   | 9.0            |
| Electrocatalysis             | 166   | 8.3            |
| Magnetic / magnetocaloric    | 154   | 7.7            |
| Hydrogen storage             | 143   | 7.1            |
| Corrosion-resistant coatings | 126   | 6.3            |

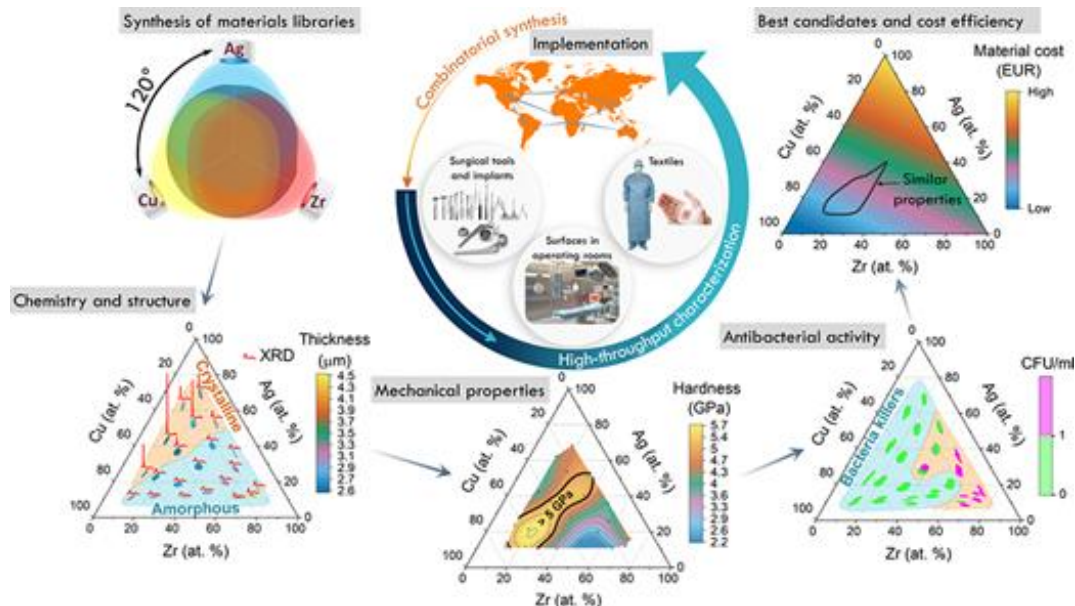
# Combinatorial thin film libraries for high-throughput alloy screening



<https://www.empa.ch/web/s206/thin-films-and-extreme-mechanical-properties>  
<https://doi.org/10.1021/acsami.4c14689>

**SwissMapper** integrates

- X-ray diffraction (XRD) - structural analysis;
- X-ray fluorescence (XRF) - composition;
- Nano-indentation - mechanics;
- Four-point probe - electrical conductivity;
- Optical microscopy - surface morphology.



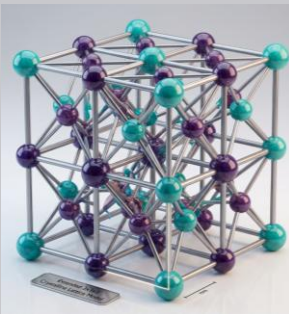
# Simulations can accelerate materials discovery



## Robust Atomistic Codes



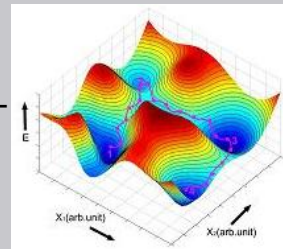
Mature simulation engines  
provide a reliable  
foundation for executing  
complex workflows.



Structural optimization:

- Conjugate gradient (CG)
- Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm
- FIRE

...



Elastic properties:

$$C_{ijkl} = \frac{\partial^2 W}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}}$$

$$K_V = \frac{(C_{11} + C_{22} + C_{33}) + 2(C_{12} + C_{13} + C_{23})}{9}$$

$$G_V = \frac{(C_{11} + C_{22} + C_{33}) - (C_{12} + C_{13} + C_{23}) + 3(C_{44} + C_{55} + C_{66})}{15}$$

Thermal properties:

Quasi-harmonic approximation (QHA)

$$F_{\text{vib}}(V, T) = \sum_{\mathbf{q}, s} \left[ \frac{1}{2} \hbar \omega_{\mathbf{q}s}(V) + k_B T \ln \left( 1 - e^{-\hbar \omega_{\mathbf{q}s}(V)/k_B T} \right) \right]$$

$$B(T) = V \left. \frac{\partial^2 G}{\partial V^2} \right|_{V(T)}$$

$$\alpha(T) = \frac{1}{V} \left( \frac{\partial V}{\partial T} \right)_P$$

$$C_p(T) = -T \left( \frac{\partial^2 G}{\partial T^2} \right)_P$$

# Large language models bring opportunities



## LLMs are no longer only question-answering systems



Natural-language interaction



Tool calling



Workflow planning

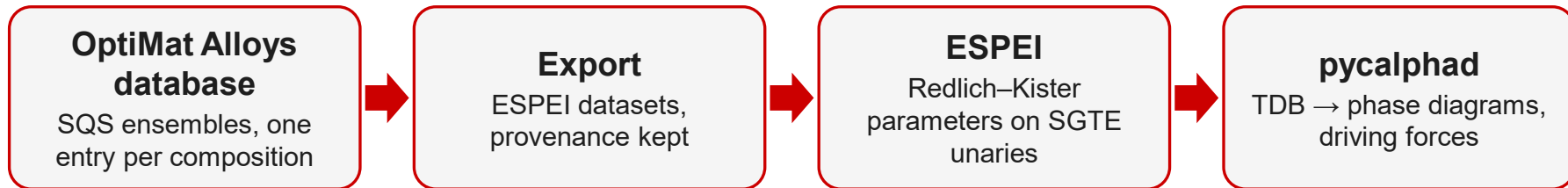


Scientific interpretation



Provenance-aware reporting

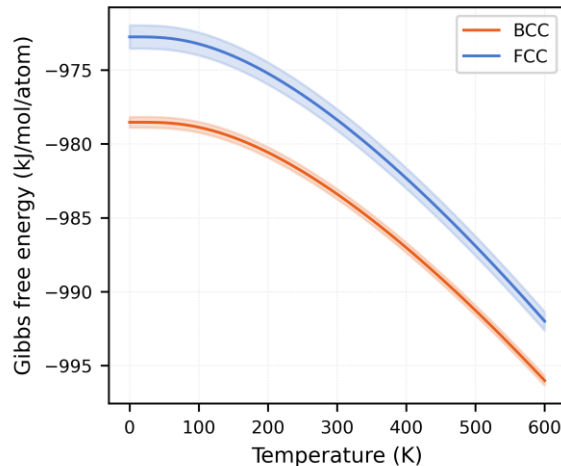
# Planned: integrate open CALPHAD workflows



## A substitutional solution phase is fitted to

- $\Delta H_{\text{mix}}$  at 0 K from SQS; excess S and Cp from quasi-harmonic G(T); molar volume  $V_m(T)$
- Ensemble mean  $\pm$  std over independent SQS cells, with calculator, version and settings recorded
- Datasets are exported, not just the fitted TDB — the fit can be repeated as potentials improve

(a) 7.6Co-19.3Cr-8.4Fe-20.7Mo-9.1Ni-34.9W (at.%)



QHA Gibbs energy, 15 SQS cells per phase, MACE omat-0; bands  $\pm 1$  std