Seitz-Invariant Prediction of Electron Localization Functions from Superposed Atomic Densities via a 3D CNN

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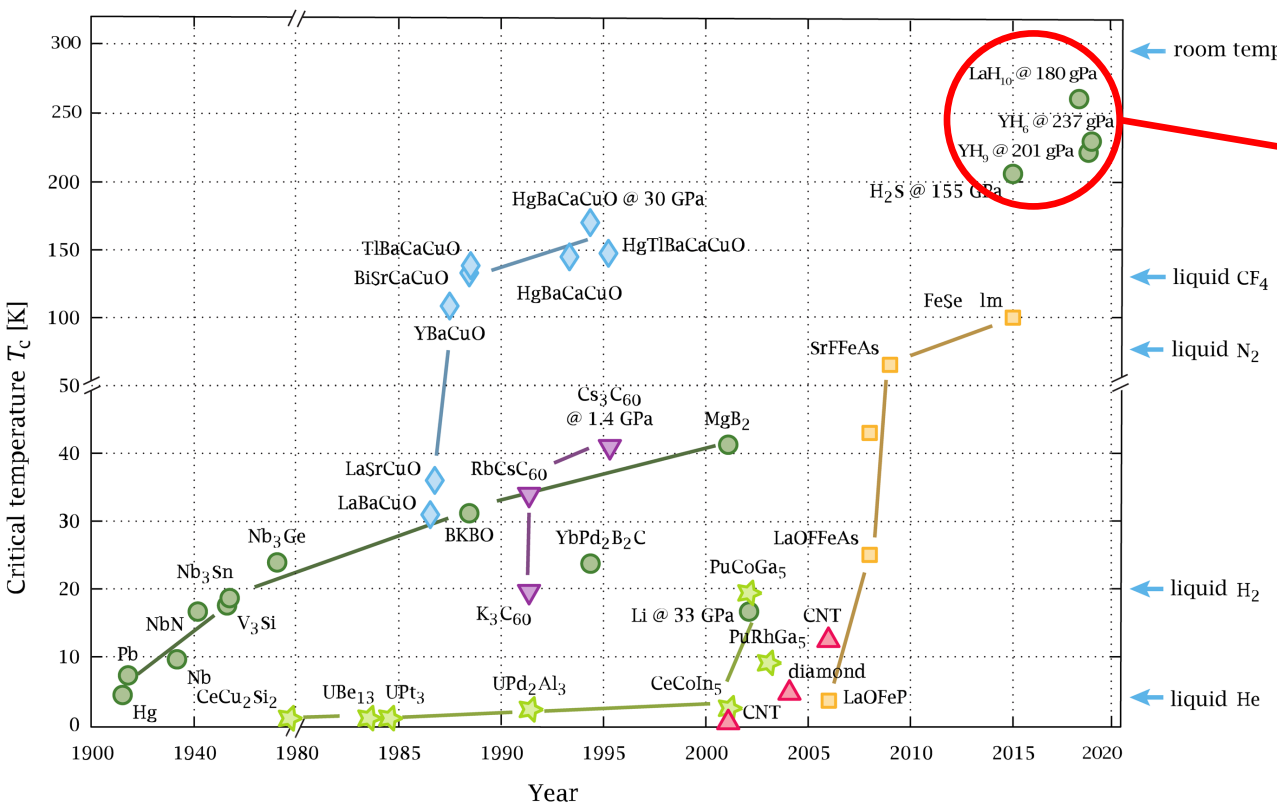
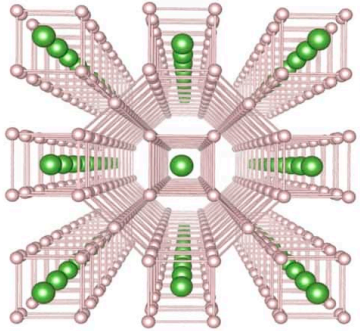
Superhydrides hold record critical temperatures





High-pressure chemistry unveils unique material structures leading to discoveries of unusual stoichiometries

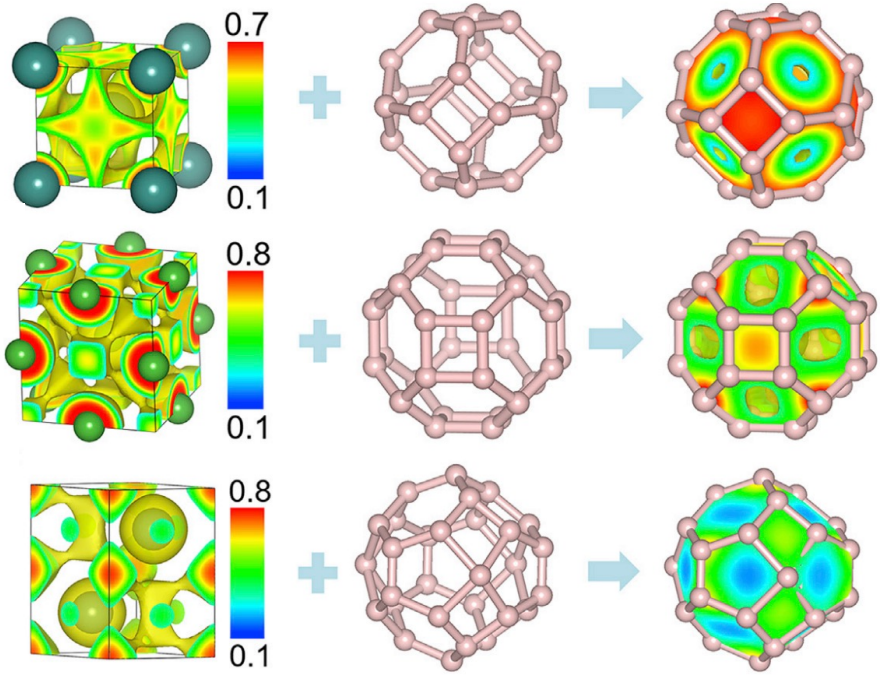
The ELF reveals superhydride formation

Electron localization function (ELF) compares local kinetic energy density to a homogeneous gas

$$\mathrm{ELF}(\mathbf{r}) = \frac{1}{1 + \chi_\sigma^2(\mathbf{r})}$$

High ELF = localized electrons
Low ELF = delocalization

Hydrogen atoms assemble in interstitial sites with high localization

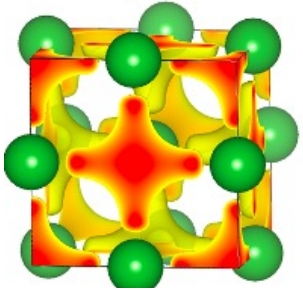


Sun & Miao, *Chem* **2023**, *9*, 443–459.

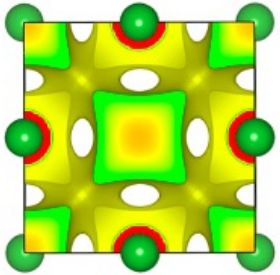
Chemical templates that assemble superhydrides

Crystal orbitals at Γ point of La lattice in LaH_{10} at 300 GPa

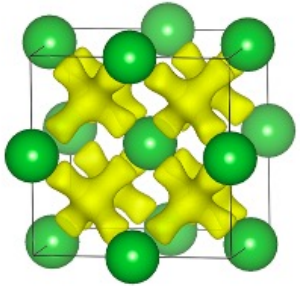
HOMO



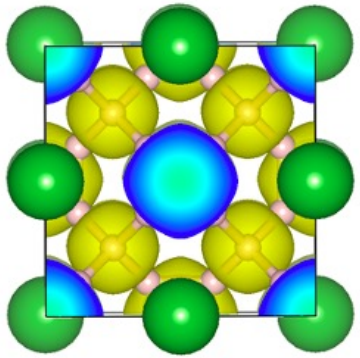
HOMO-1



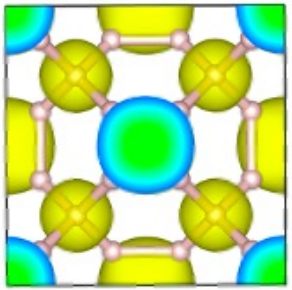
HOMO-2



HOMO at Γ point of LaH_{10} at 300 GPa



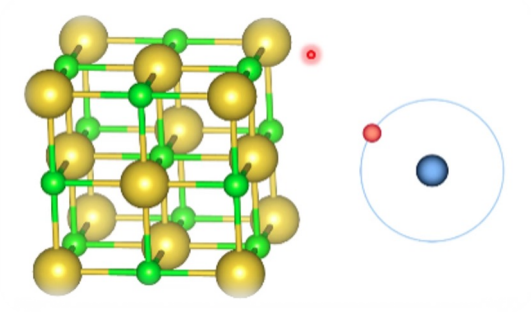
LUMO at Γ point of H lattice in LaH_{10} at 300 GPa



Interstitial electrons in metal lattices naturally occupy H lattice orbitals

The ELF can be expensive to calculate

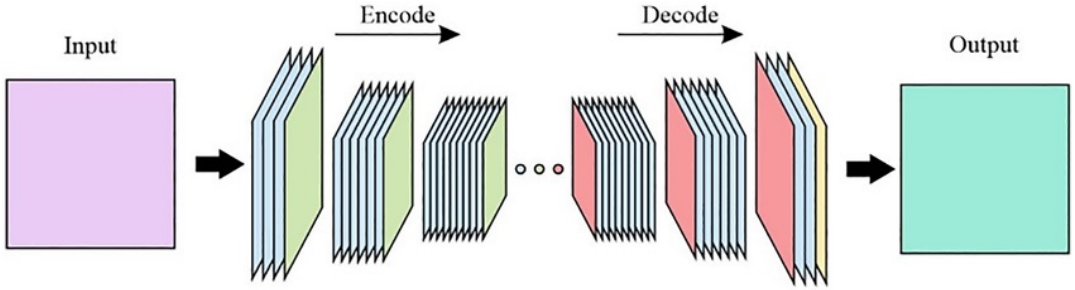
First Principles (QM)



$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi$$

The time required to run a quantum mechanics-based calculation scales cubically with electron count (N)

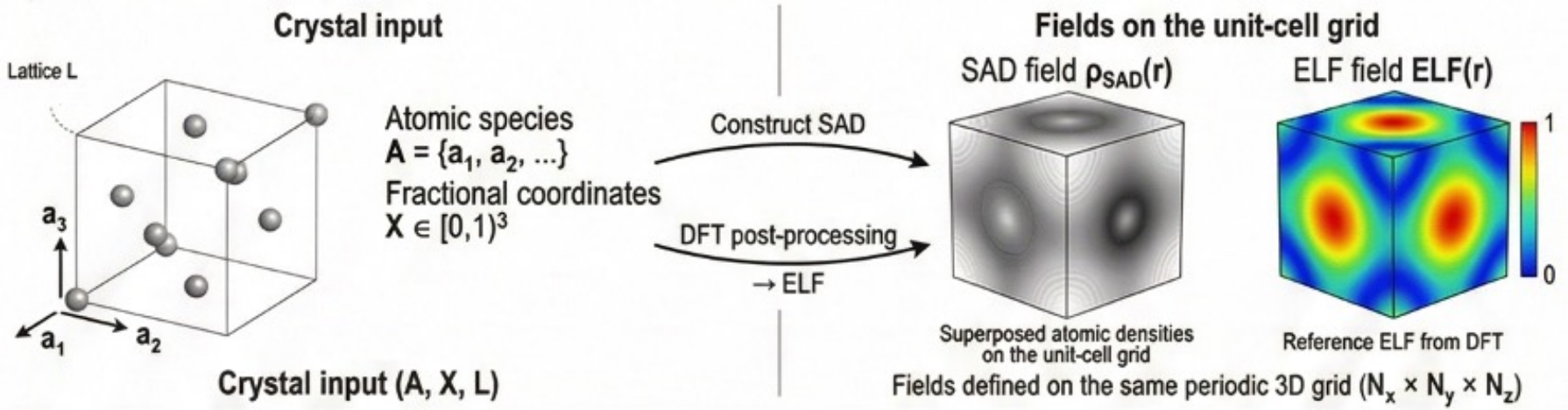
Machine Learning (ML)



Solution: We can **treat the ELF as a 3D image** and train a model to predict it directly

Problem: How do we represent our structure?

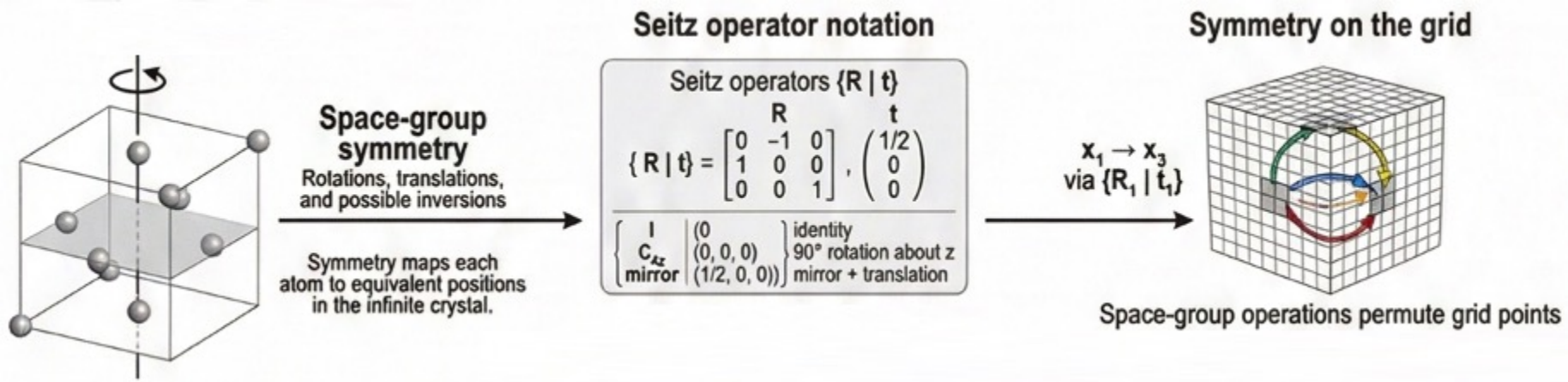
Crystal structure representation



SAD is the electron density obtained by freezing atomic charge density at each atom center without allowing their electron clouds to hybridize or relax into bonded states

Since the SAD and ELF have the same grid size, the **problem is now an image transformation**

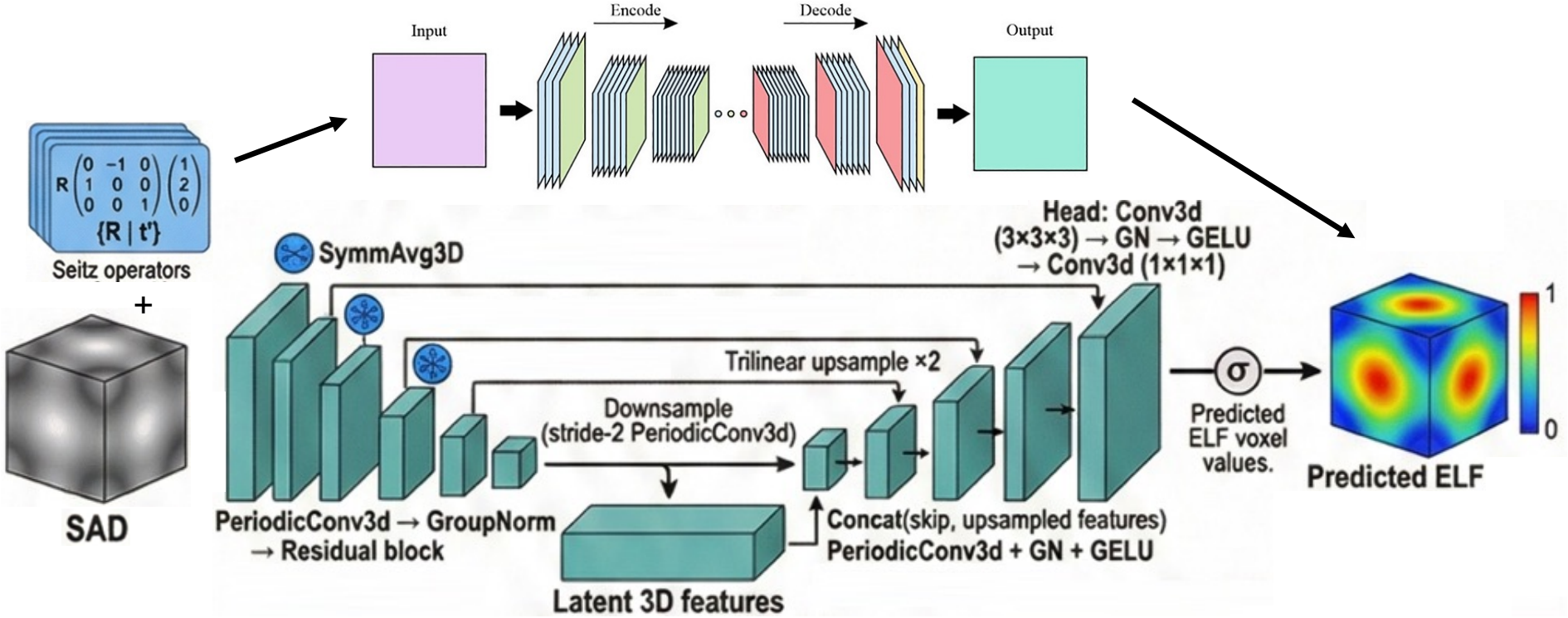
Making the model Seitz-Invariant



Seitz symmetry – Standard notation system for describing the symmetry operations of crystal structures in 3D space groups

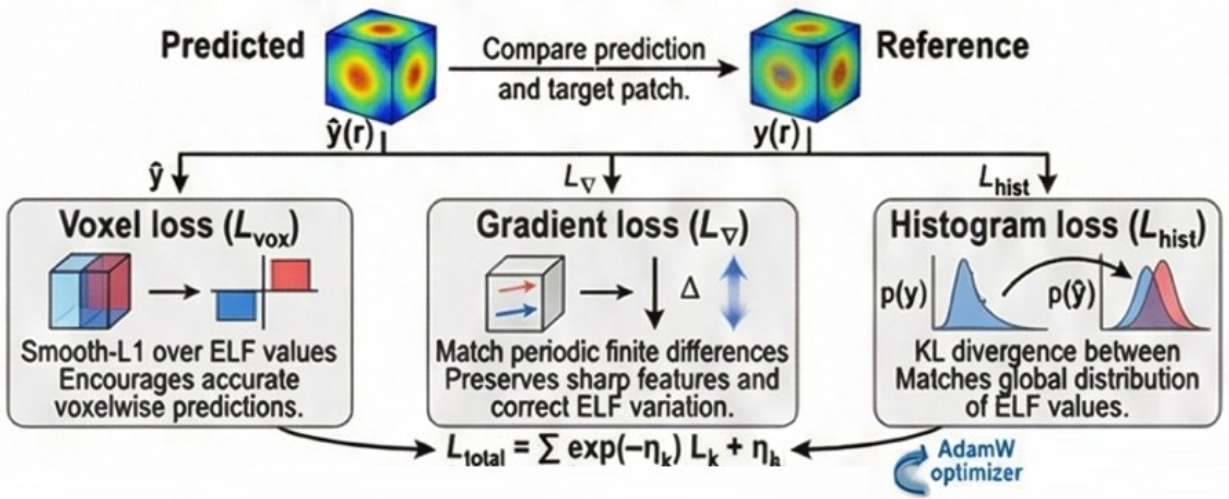
Invariance – Property that guarantees the model makes the same prediction even if the crystal structure is rotated or translated according to its symmetry group

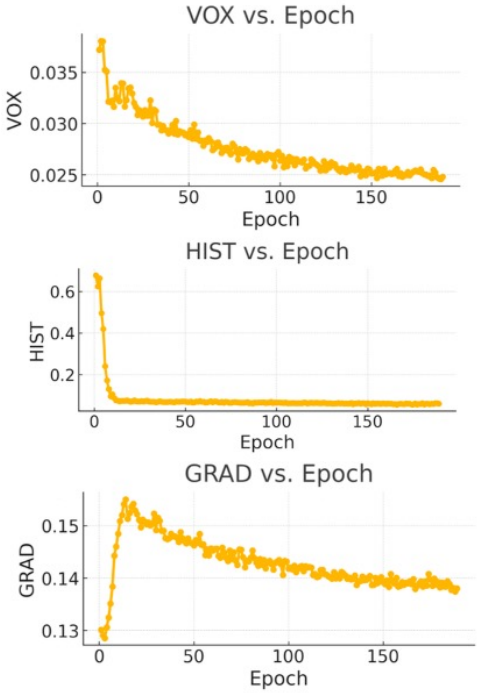
Architecture for a symmetry-aware image transform



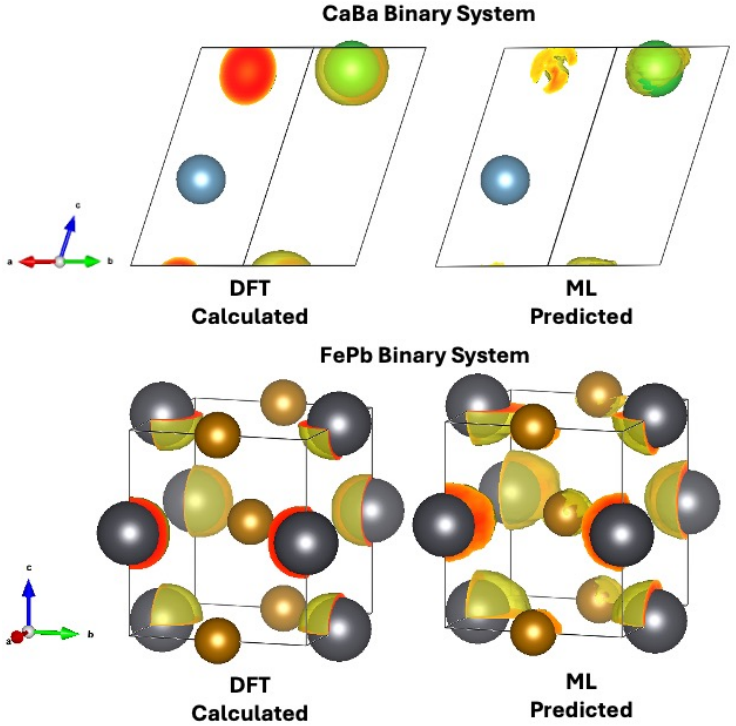
Physics-aware loss function

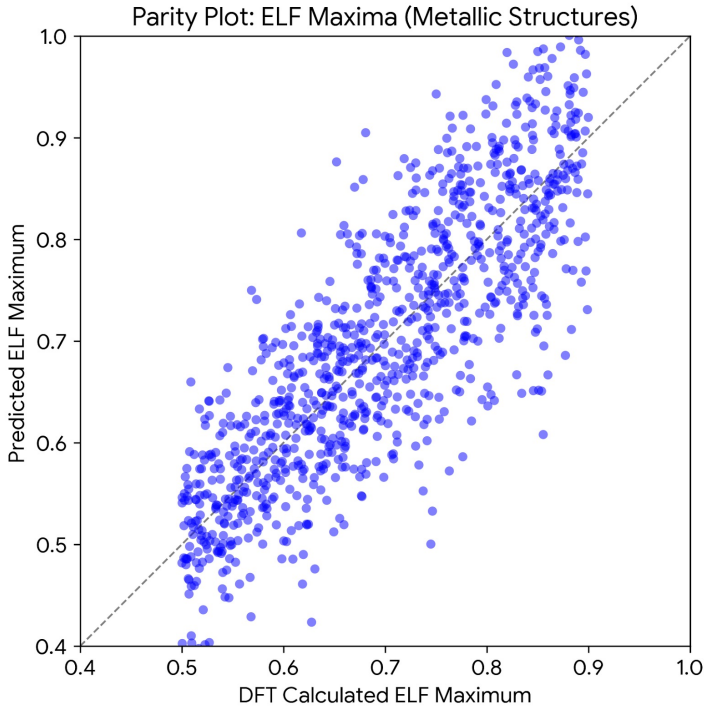
Kendall Loss: An adaptive weighting scheme that automatically learns how to balance the voxel, gradient, and histogram objectives during training, eliminating the need to manually tune loss weights.





Successful ELF Prediction





Model tested on subset of metal lattices

Maxima most relevant to prediction of superhydride structures

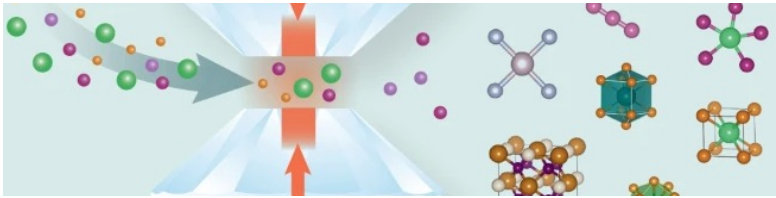
Conclusion

Novel Contributions

- **3D image transformation** bypasses quantum mechanics calculations
- **SAD representations** are used to represent 3D crystals
- **Seitz-Invariance** guarantees predictions respect crystal symmetry
- **Physics-aware optimization** via Kendall loss automatically balances training objectives

Next Steps

- **Extend training set** beyond metals so the SAD→ELF operator supports more chemical space
- **Generate compressed ELFs** to train model on high-pressure regimes
- Use high-pressure model to rapidly evaluate metal lattice ELFs to **discover novel superconductors**



Acknowledgements

Team

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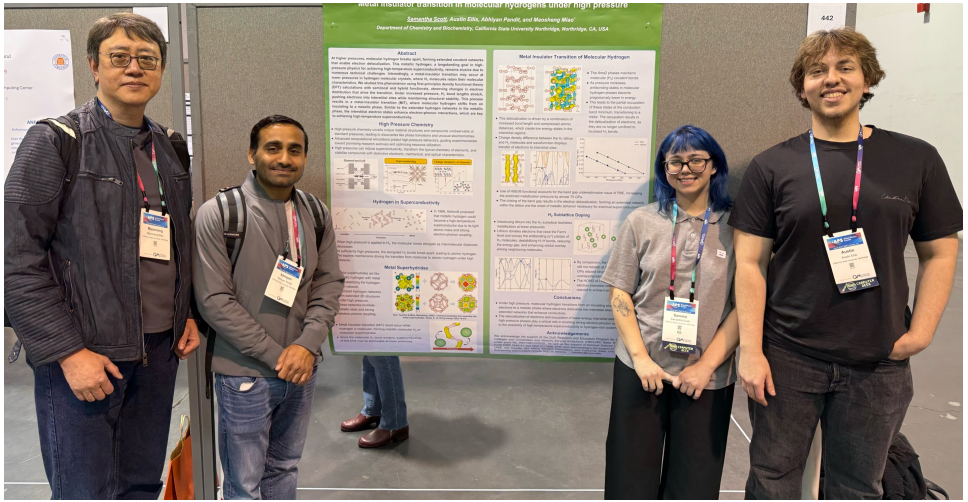

Check out the paper!

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MAJOR RESEARCH INSTRUMENTATION

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