Symmetry-Aware Prediction of Electron Localization Functions from Superposed Atomic Densities

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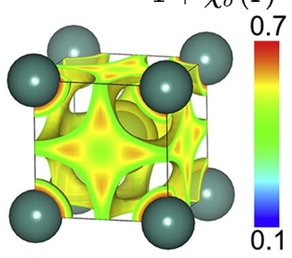
Abstract

The electron localization function (ELF) is a key diagnostic of bonding and electronic structure across materials, including high-pressure regimes. However, predicting ELF directly from composition and crystal structure is difficult because it is highly non-linear. We develop a deep learning model that transforms a 3D superposition of atomic densities (SAD) into ELF on the unit-cell grid. Because SAD is evaluated in the actual lattice, the representation can implicitly include pressure and can rapidly score candidate metal sublattices (templates) for compressed compounds. Our architecture is a periodic 3D U-Net with circular padding, explicit space-group symmetry pooling using Seitz operators in the local patch frame, and memory-efficient training on periodic patches with epoch-wise origin jitter. Trained on 50,000 metal-only structures, the model is symmetry-aware at both data and network levels and is designed to scale to large unit cells without significant memory cost.

Background

Electron Localization Function

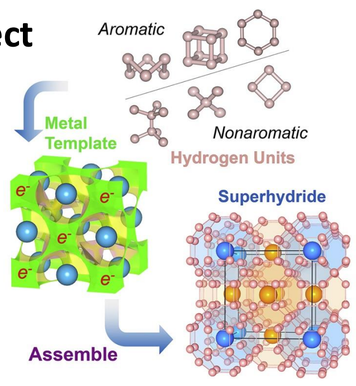
$$\mathrm{ELF}(\mathbf{r}) = \frac{1}{1+\chi_\sigma^2(\mathbf{r})}$$



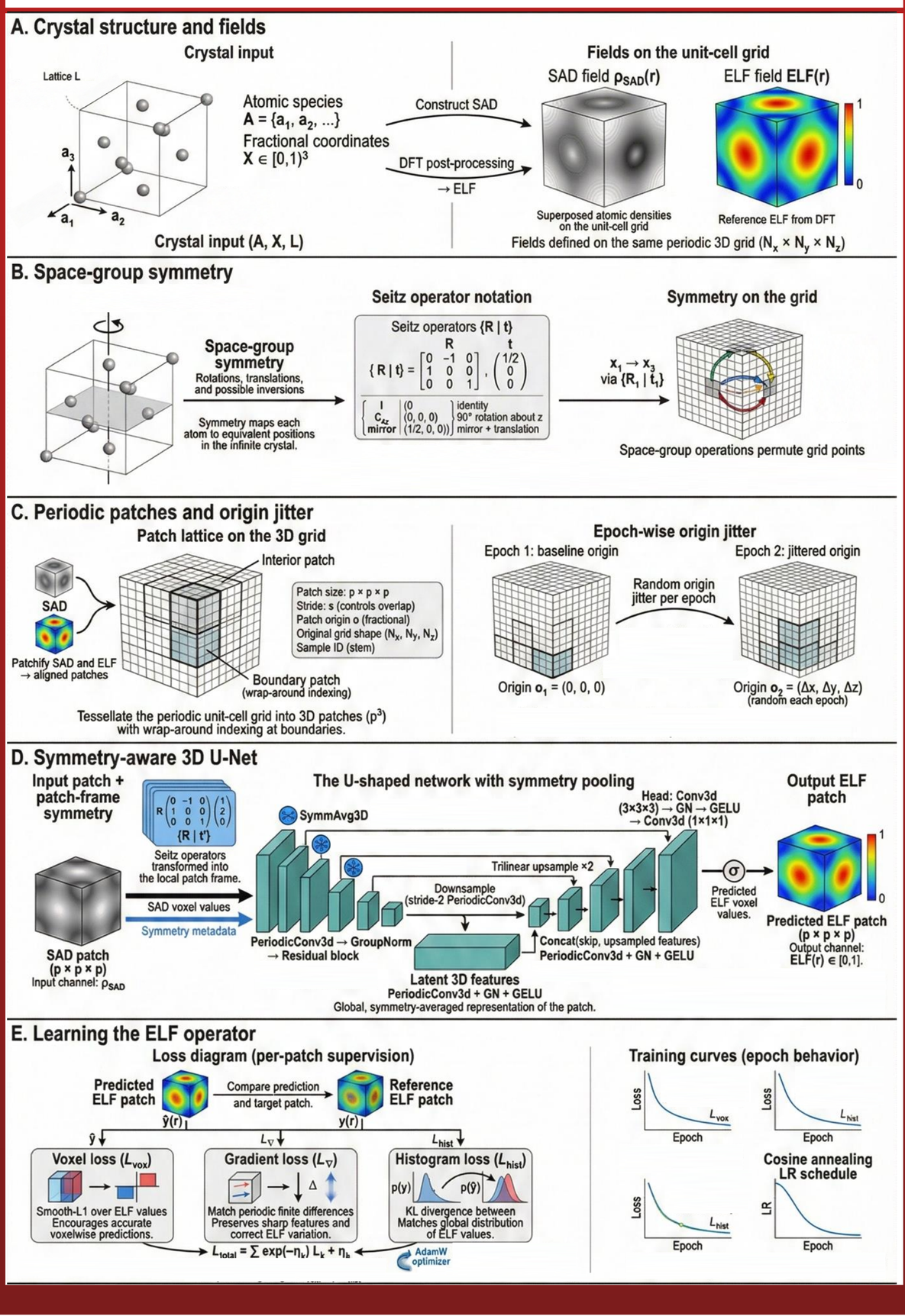
- ELF is computed from a dimensionless quantity that compares the local kinetic-energy density of electrons to a homogeneous electron gas
- High ELF values highlight regions of localized electrons like bonds, lower ELF values indicate more delocalized or metallic electrons

Chemical Template Effect

- Electrons occupying the quantum orbitals at the interstitials of metal sublattices form a template that assembles non-metal lattices
- Method based on template theory significantly improves the efficiency of searching for new complex superhydrides

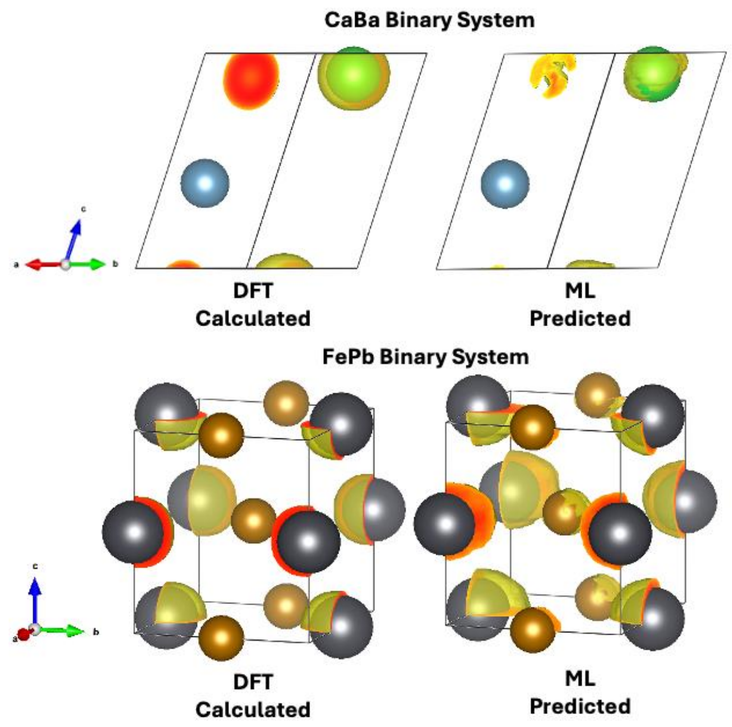


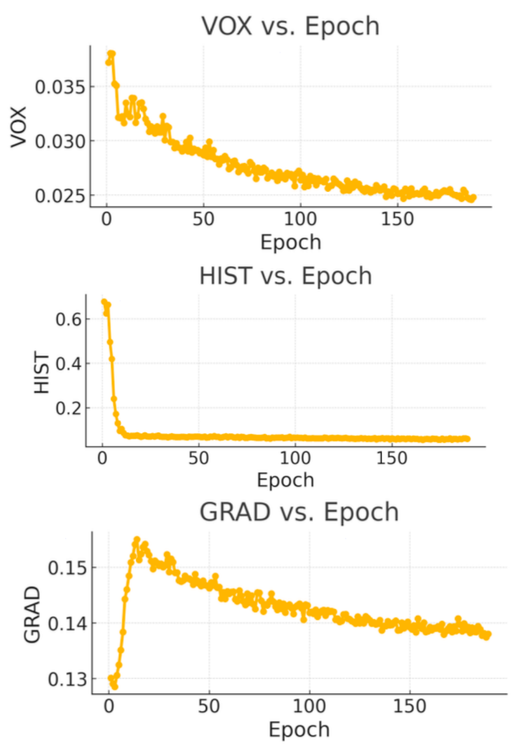
Methods and Workflow



Results

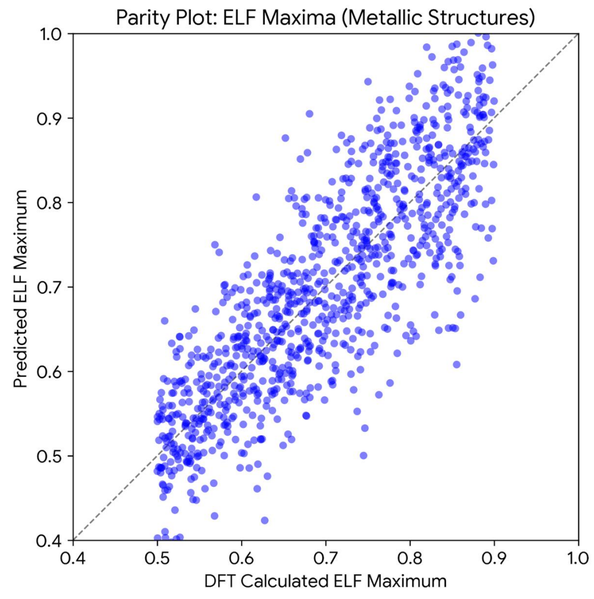
- DFT and ML ELF isosurfaces for the CaBa and FePb binary systems show nearly identical localization basins around corresponding Ba and Pb atoms, with slight hallucination on the Fe atoms
- The model reproduces both the shape and relative intensity of high-ELF lobes, indicating that it captures the same bonding picture as the reference DFT ELF





- The VOX term decreases steadily, showing that the network is learning point-wise ELF values across the grid
- The HIST term drops sharply within the first few epochs and quickly plateaus, meaning the global ELF histogram is matched early in training
- The GRAD term exhibits a modest initial rise as the uncertainty-weighted loss terms rebalance, then decays to a stable plateau, indicating smooth, physically consistent ELF fields

- The parity plot of ELF maxima over the metallic test set shows points tightly clustered along the y = x line, demonstrating strong agreement between predicted and DFT ELF extrema
- Scatter remains small across the full range of ELF maxima suggesting model transfers well to unseen crystal chemistries and symmetries



Conclusions and Perspectives

- We constructed a symmetry-aware, periodic 3D U-Net that maps pressure-implicit SAD fields to ELF, trained on 50,000 metal-only structures
- Reproduces DFT ELF across diverse metallic crystals while remaining fast enough for inner-loop template screening.
- Extend the training set beyond metals so the learned SAD→ELF operator can support a wider range of materials projects and chemistries.
- Generate compressed structures and corresponding DFT ELFs to explicitly train the model on high-pressure regimes
- Use the high-pressure model to rapidly evaluate metal-sublattice ELF and template strength, enabling fast screening of candidate metal superhydrides and related high-pressure materials.

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