

STRUCTURE GENERATION



CANDIDATE SPACE

1. CANDIDATE ACQUISITION

Sampling top N polymorphs from candidate space by weighting energy prediction & uncertainty



5. ENERGY PREDICTIONS

ML model estimates of formation energy and model uncertainty of "unseen" candidates



ACTIVE LEARNING

2. FIRST-PRINCIPLES CALCULATIONS

Structural relaxation of candidates to local energy minima (ΔH_f) by performing ab-initio DFT simulations



4. MACHINE LEARNING SURROGATE MODEL

Building surrogate ML models for polymorph stability by training on acquired DFT data



3. STRUCTURAL FINGERPRINTS

Encoding chemical and structural information into a fingerprint vector via Voronoi tessellation

