STRUCTURE GENERATION

CANDIDATE SPACE

ACTIVE LEARNING

1. CANDIDATE ACQUISITION

Sampling top N polymorphs from candidate space by weighting the surrogate model's energy prediction & uncertainty

5. ENERGY PREDICTIONS

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

2. FIRST-PRINCIPLES CALCULATIONS

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

3. STRUCTURAL FINGERPRINTS

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

4. MACHINE LEARNING SURROGATE MODEL

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