STRUCTURE GENERATION

CANDIDATE SPACE

ACTIVE LEARNING

1. CANDIDATE ACQUISITION
Sampling top polymorphs from candidate space by weighting the surrogate model's energy prediction & uncertainty

5. ENERGY PREDICTIONS
ML model estimates formation energy and model uncertainty of "unseen" structural 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