

STRUCTURE GENERATION

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



ACTIVE
LEARNING

2. FIRST-PRINCIPLES CALCULATIONS

Structural relaxation of candidates to local energy minima 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



CANDIDATE
SPACE