

Candidate Space Generation

Materials databases

- ▼ Select desired stoichiometry
- ▼ Filter for structural uniqueness
- ▼ Replace elements with desired
- ▼ Pre-optimize cell volume

Final candidate structures

Seed with random DFT

Active Learning Search

ML
Training

Predict ΔE_f

Acquisition/DFT

STOP

Yes

No

New stable
structures
found?