

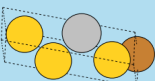
Binaries

SNAP Ensemble
Training

SNAP 1 SNAP 2 SNAP 3 SNAP 4 SNAP 5

× 5

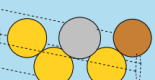
Single Unrelaxed
Compound



Relax

SNAP 1 SNAP 2 SNAP 3 SNAP 4 SNAP 5

Single Relaxed
Compound



Predict

SNAP 1 SNAP 2 SNAP 3 SNAP 4 SNAP 5

E, σ

$\min \sigma$

$\leq \sigma_{\text{cut}}?$

Convex Hull
Sampling

Binary
Prototypes

Stoichiometry Selection

enumlib

Volume Scaling

Ternary
Candidates

SNAP Screening

Energy Ranking

Best
Ternaries

DFT Relaxation

Single Best
Ternary

Convex
Hull

