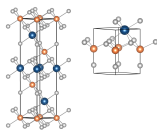
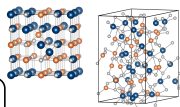


DFT reference dataset

Ordered configs.



Defective & disordered configs.



DFT calculations

ML Potential



Energy
Forces
Stresses

Train MLP model

Large-scale MD
simulations

Structural dynamics

Disordering dynamics
Mechanical response
Coordination transition

DL Hamiltonian

Hamiltonian
matrix elements



Train DLH model

Predict Hamiltonians

Electronic structure

Unfold band structure
Charge distribution
Orbital coupling

Representative
snapshots

Origin of disorder stability & electronic structure