

ANNN Potential Construction

generate.x

Transform atomic coordinates to invariant representation of the local atomic environments.

Env. Setups
for each atomic species

Reference Set:
atomic structures and energies

Training Set File
atomic environm. and setups

train.x

ANN Potentials
for each atomic species

Optimize network weights according to selected method (on-line or batch training).

PARALLEL

predict.x

Transform atomic coordinates
PARALLEL

Atomic Structure

ænetLib

Evaluate atomic energies & forces
PARALLEL

total energy & atomic forces

Application