

Create sytem
(with orthorhombic
unit cell)

Perform Geometry
minimisation

Sample velocities
at 300K

Legend

NVT simulations

NPT simulations

Equilibrate at
300K

Linearly increase
temperature to
800K

Equilibrate at
800K

Linearly decrease
temperature to
300K

Equilibrate at
300K

Equilibrate at
300K under NVT