

Phase Diagram

Heat Capacity
Profiles (C_V)

Melting
Curves

Umbrella
Sampling
Monte Carlo
(USMC)

Wang-Landau
Monte Carlo
(WLMC)

Markov-Chain
Monte Carlo
(MCMC)

Configurations

Free Energy Analysis

Expanded Ensemble
Density of States
(EXEDOS)

Multidimensional
Lowest Energy
Algorithm (MULE)

2D Free Energy
Landscapes (FELs)

Minimum Free
Energy Path (MFEP) &
Barrier Heights (ΔF^\ddagger)

