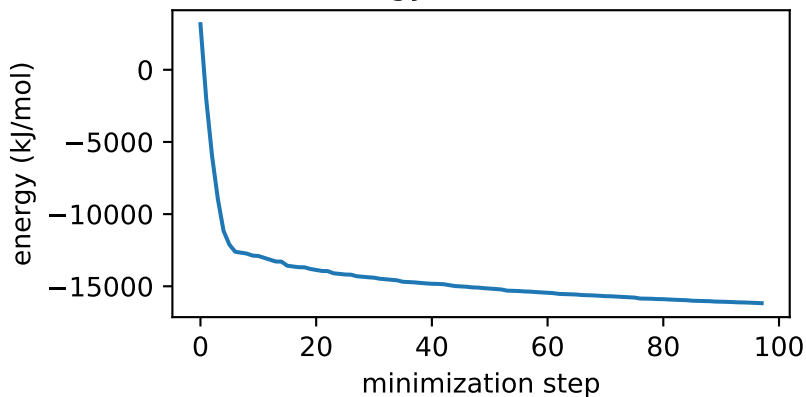
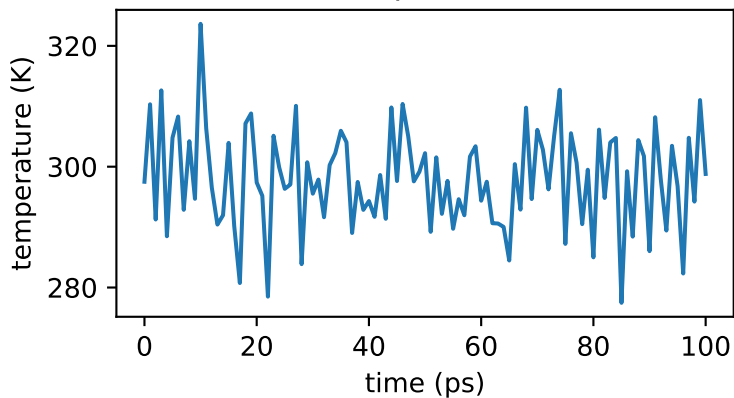


energy minimization



NVT equilibration



NPT equilibration

