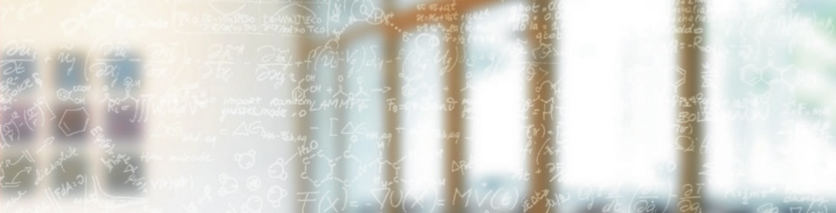
import random
LAMMPS
F(X) = -∇U(X) = MV(t)
qtot
BOLD