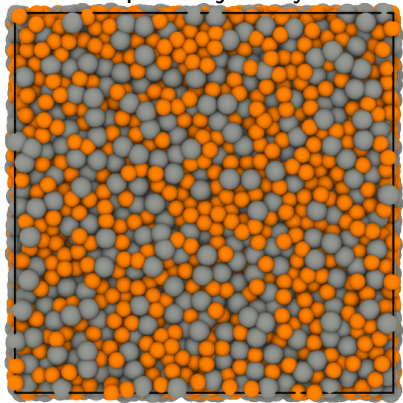


(a)

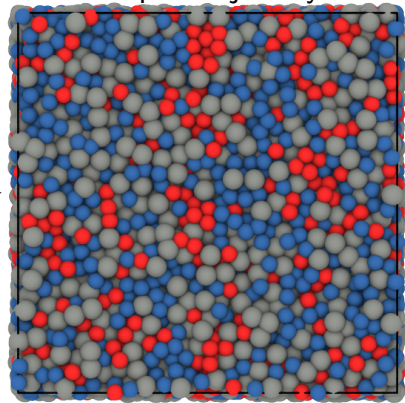
input trajectory



pySCL

(b)

output trajectory



(c)

Bond angle distributions

