QUICK-SHEET for molsim

Action	Specifier	Input values	Output values
load	**xyz**	**File name (string)**	
	top	**File name (string)**	
save		**1 Types (string)** **2 File name (string)**	
set	**timestep**	**Time step (scalar – default 0.005)**	
	temperature	**Temperature (scalar – default 1.0)**	
	cutoff	**Max. cutoff (scalar – default 2.5)**	
	omp	**No. threads (int scalar – default 1)**	
	exclusion	**'bonded' or 'molecule'** **(string – default 'all')**	
	temperaturerelax	**Temp. relaxation time** **(scalar – default 0.01)**	
	compressionfactor	**Compression factor** **(scalar – default 0.99995)**	
	types	**Particle types (string)**	
	skin	**Buffer-skin for neighbourlist** **(scalar – default 0.25)**	
	charges	**Atom charges (vector)**	
	lattice	**1 Part. dimensions (int array length 3)** **2 Box dimensions (array length 3)**	
	molconfig	**1 xyz file (string)** **2 top file (string)** **3 Numb. of molecules** **4 Crystal initial density** **5 Random seed (int)**	
get	**numbpart**		**Scalar**
	box		**Vector**
	energies		**Vector (E_{kin}, E_{pot})**
	velocities		**Matrix**
	positions		**Matrix**
	forces		**Matrix**
	types		**String**
	molpositions		**Matrix**

	pressure	Scalar

calcforce	lj	1 Types (string) 2 Cutoff (scalar) 3 σ (scalar) 4 ε (scalar) 5 aw (scalar)
	bond	1 Bond type (int scalar) 2 Bond length (scalar) 3 Spring constant(scalar)
	angle	1 Angle type (int scalar) 2 Eq. angle (scalar) 3 Spring constant (scalar)
	torsion	1 Torsion type (int scalar) 2 Potential parameters (vector)
	coulomb	1 Algorithm (“sf” or “wolf”) 2 Cutoff (scalar) 3 <OPT for “wolf”:> Screening (Scalar)
	lattice	1 Particle type (string) 2 Spring constant (scalar)
	dpd	1 Types (string) 2 Cutoff (scalar) 3 Repulsion parameter (scalar) 4 σ (scalar)

integrate	leapfrog	
	dpd	λ (scalar)

thermostate	relax	1 Particle type (string) 2 Temperature (scalar) 3 Thermostat relax time (scalar)
	nosehoover	1 Particle type (string) 2 Temperature (scalar) 3 Thermostat mass (scalar)

sample	vacf/mvacf	1 Length vector (int scalar) 2 Time span (scalar)
	sacf/msacf	1 Length vector (int scalar) 2 Time span (scalar)
	hydrocorrelations/ mhydrocorrelations	1 Length vector (int scalar) 2 Time span (scalar) 3 No. wavevectors (int scalar)
	profiles	1 Particle type (string) 2 Length vector (int scalar) 3 Sample freq. (int scalar)
	msd	1 Length vector (int scalar)

		2 Time span (scalar) 3 No. wavevectors (int scalar) 4 Particle type (string)
	do	
task	lj	1 Types (string) 2 Cutoff (scalar) 3 σ (scalar) 4 ε (scalar) 5 Block no.
	bond	1 Bond type (int scalar) 2 Bond length (scalar) 3 Spring constant(scalar) 4 Block no.
	angle	1 Angle type (int scalar) 2 Eq. angle (scalar) 3 Spring constant (scalar) 4 Block no.
	torsion	1 Torsion type (int scalar) 2 Potential parameters (vector) 3 Block no.
	coulomb	1 Cutoff (scalar) 2 Block no.
	do	1 Total no. blocks

compress		Target density

add	force	1 Forces (vector) 2 Direction (int scalar)
	tolattice	1 dx (scalar) 2 Direction (int scalar)

clear

print
reset