Unit 14 - Week 9

Assignment 9

The due date for submitting this assignment has passed.
As per our records you have not submitted this assignment.

Due on 2020-04-01, 23:59 IST.

1) True or False: *2 points*

In molecular dynamics, instead of computing the time averages, we calculate the phase averages.

- True
- False

No, the answer is incorrect.
Score: 0
Accepted Answers:
False

2) For a commonly used expression for the Lennard-Jones potential given by the equation *2 points*

$$\phi(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{X} - \left(\frac{\sigma}{r}\right)^{Y}\right]$$

X , Y are most likely

- 12,6
- 6,12
- X - Y = 5
- X - Y must always be 6

No, the answer is incorrect.
Score: 0
Accepted Answers:
12,6

3) _____ are files which contain snapshots of atoms and various per-atom values and are written at a specified frequency. *2 points*

- Dump files
- Restart files
- Data files
- Input files

No, the answer is incorrect.
Score: 0
Accepted Answers:
Dump files

4) Periodic boundary conditions (PBC) are used in molecular dynamics simulations to avoid problems with boundary effects caused by finite size, and make the system more like an infinite one *2 points*

- True
- False

No, the answer is incorrect.
Score: 0
Accepted Answers:
True

5) In LAMMPS, the forces on each atom in the system is calculated by multiplying the mass of the atom by the acceleration of the atom *2 points*

- True
- false

No, the answer is incorrect.
Score: 0
Accepted Answers:
false

6) _____ are mathematical functions for calculating the potential energy of a system of atoms with given positions in space. *2 points*

- Interatomic potentials
- Group functions
- Math functions
- Atom functions

No, the answer is incorrect.
Score: 0
Accepted Answers:
Interatomic potentials

7) What is the expression for Buckingham potential ? *2 points*

- $\phi = -Ae^{Br} + \frac{-C}{r^6}$
- $\phi = -Ae^{-Br} + \frac{C}{r^6}$
- $\phi = Ae^{-Br} - \frac{C}{r^6}$
- $\phi = Ae^{-Br} + \frac{C}{r^6}$

No, the answer is incorrect.
Score: 0
Accepted Answers:
$\phi = Ae^{-Br} - \frac{C}{r^6}$

8) In LAMMPS input script file, any line ending with a '&' is a comment. *2 points*

- True
- False

No, the answer is incorrect.
Score: 0
Accepted Answers:
False

9) In LAMMPS input script file, _____ command creates a simulation box based on the specified region. *2 points*

- box
- create_box
- region
- fill_box

No, the answer is incorrect.
Score: 0
Accepted Answers:
create_box

10) Which of the following commands is always needed for a LAMMPS input script to run successfully *2 points*

- run
- dump
- units
- create box

No, the answer is incorrect.
Score: 0
Accepted Answers:
units

11) Which of the following commands will output information pertaining to the simulation box *2 points*

- fix
- dump
- thermo
- region

No, the answer is incorrect.
Score: 0
Accepted Answers:
thermo