

Unit 6 - Week 1

Course outline

How does an NPTEL online course work?

MATLAB

MATLAB_SCRIPTS

LAMMPS_SCRIPTS

Installation_Procedure

Week 1

- Introduction to the course
- Some applications of MD simulations
- Introduction to Bravais lattices and constructing simple crystals with MATLAB
- Introduction to symmetry - 1
- Symmetry Elements - 1
- Quiz : Assignment 1
- Lecture materials for week 1
- Week 1 Feedback :Foundations of Computational Materials Modelling

Week 2

Week 3

Week 4

Week 5

Week 6

Week 7

Week 8

Week 9

Week 10

Week 11

Week 12

Additional Documents

Download videos

Text Transcripts

Assignment 1

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

Due on 2020-02-12, 23:59 IST.

1) How many Bravais Lattice are there in 3D?

2 points

- 10
 12
 14
 8

No, the answer is incorrect.
Score: 0
Accepted Answers:
14

2) Fill in the blanks:

_____ is an infinite array of discrete points with an arrangement and orientation that appears exactly the same from any point.

No, the answer is incorrect.
Score: 0
Accepted Answers:
String starting with: Bravais Lattice
String starting with: BravaisLattice

2 points

3) Fill in the blanks:

_____ is the set of operations including translations that leave the crystal as it is.

No, the answer is incorrect.
Score: 0
Accepted Answers:
String starting with: Space group
String starting with: Spacegroup

2 points

4) A crystal is a combination of lattice and basis.

2 points

- True
 False

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

5) Orthorhombic bravais lattice has the following: $a \neq b = c$ and $\alpha = \beta = \gamma = 90^\circ$

2 points

- True
 False

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

6) Penrose-tiling has 4 fold symmetry but no translational symmetry. (Use the internet to know what is Penrose tiling)

2 points

- True
 False

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

7) The diamond structure is an _____ lattice.

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: String) FCC
(Type: String) Face centred cubic
(Type: String) Face-centered cubic

0 points

8) The diamond structure is having _____ basis atoms

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: Numeric) 2

0 points

9) What is the bravais lattice of a sheet of graphene?

2 points

- Orthorhombic
 Tetragonal
 Hexagonal
 Graphene has a hexagonal net structure, it is not a Bravais lattice

No, the answer is incorrect.
Score: 0
Accepted Answers:
Graphene has a hexagonal net structure, it is not a Bravais lattice

10) A non-primitive unit cell is the one that contains only a one lattice point.

2 points

- True
 False

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

11) A motif is a group of atoms attached to every lattice point.

2 points

- True
 False

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

12) In two dimensions, there are _____ unique ways you can arrange a set of points such that no matter from which point you look, it is exactly the same.

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: Numeric) 5

2 points

13) Given that \hat{i} , \hat{j} , and \hat{k} are the unit normal vectors of the Cartesian - coordinate system. Three lattice vectors can be written as: $a_1 = a\hat{i}$, $a_2 = b\hat{j}$ and $a_3 = c\hat{k}$, where a , b and c are lattice constants. The expression $R = n_1a_1 + n_2a_2 + n_3a_3$, where n_1 , n_2 and n_3 are integers generates a _____

2 points

- Cubic lattice
 Orthorhombic lattice
 Tetragonal lattice
 Hexagonal lattice

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

14) If vectors $a = a\hat{i}$, $b = b\hat{j}$ and $c = c\hat{k}$ form a primitive set of lattice vectors, the unit cell has

2 points

- 4 lattice points
 1 lattice point
 3 lattice points
 2 lattice points

No, the answer is incorrect.
Score: 0
Accepted Answers:
1 lattice point

15) Fill in the blanks:

All crystals, possessing the same symmetry elements belong to a _____.

No, the answer is incorrect.
Score: 0
Accepted Answers:
String starting with: space group
String starting with: spacegroup

2 points