Unit 17 - Week 12

Course outline

How does an NPTEL online course work?

MATLAB

MATLAB_SCRIPTS

LAMMPS_SCRIPTS

Installation_Procedure

Week 1

Week 2

Week 3

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Week 12

- ● LAMMPS exercises 5
- ○ Quiz : Assignment 12
- ○ Week 12 Feedback : Foundations of Computational Materials Modelling

Additional Documents

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Text Transcripts

Assignment 12

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

Due on 2020-04-22, 23:59 IST.

Note : This assignment is only for practice purpose and it will not be counted towards the Final score

1) True or False: *2 points*

Radial distribution function is nothing but the relative density of atoms as function of radius.

○ True
○ False

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

2) It is useful to classify crystals based on the symmetry they possess because *2 points*

○ it is easier to visualize crystals
○ the crystal symmtery reflects in property symmetry
○ all crystals belong to some symmetry group
○ the symmetry elements are obvious

No, the answer is incorrect.
Score: 0
Accepted Answers:
the crystal symmtery reflects in property symmetry

In a orthorhombic crystal a glide plane is located at $(x, 0.4, z)$. The atom located at fractional coordinate (0.5, 0.2, 0.5) will generate the coordinate (__A__ , __B__ , __C__) as a result of a c–glide.

3) The Answer of A =_________

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: Numeric) 0.5

1 point

4) The Answer of B = _______

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: Numeric) 0.6

1 point

5) The Answer of C = ______

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: Numeric) 0
(Type: Numeric) 1

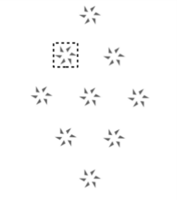
2 points

6) The screw rotation axis can replace a _______ *2 points*

○ mirror
○ glide plane
○ rotation axis
○ any symmetry operation

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

Carefully study the pattern in Figure and answer the following questions. Note that the motif which is generated by using several scalene triangles, is marked using a dashed box



7) The motif indicated by the dashed box has **2 points**

○ One mirror plane
○ Two mirror planes
○ one 6 fold rotation axis
○ One three fold axis only

No, the answer is incorrect.
Score: 0

Accepted Answers:
one 6 fold rotation axis

8) The point group of the motif indicated by the dashed box is **2 points**

○ 6
○ 6m
○ 3
○ 4m

No, the answer is incorrect.
Score: 0

Accepted Answers:
6

9) The plane group of this pattern (if repeated infintiely in the 2 directions is) **3 points**

○ p2
○ p6
○ p6m
○ p3

No, the answer is incorrect.
Score: 0

Accepted Answers:
p2

10) The scalene triangle which is used to create the motif has symmetry **1 point**

○ 3
○ 2
○ 1
○ none of the above

No, the answer is incorrect.
Score: 0

Accepted Answers:
1

11) There are _____ space groups in all.

No, the answer is incorrect.
Score: 0

Accepted Answers:
(Type: Numeric) 230

2 points

12) Statistical mechanics does not provide a connection between macroscopic and microscopic properties **2 points**

○ True
○ False

No, the answer is incorrect.
Score: 0

Accepted Answers:
False

13) In statistical mechanics, a _______ is a specific microscopic configuration of a thermodynamic system that the system may occupy with a certain probability in the course of its thermal fluctuations

No, the answer is incorrect.
Score: 0

Accepted Answers:
(Type: String) microstate

2 points

14) A mirror operation is a point operation *2 points*

○ True
○ False

No, the answer is incorrect.
Score: 0

Accepted Answers:
True

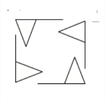
15) A primitive Tetragonal unit cell has ______ lattice points per unit cell

No, the answer is incorrect.
Score: 0

Accepted Answers:
(Type: Numeric) 1

2 points

16) The Hermann-Maugin symbols for the point groups for the pattern (Fig.below) is _____ *2 points*

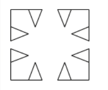


○ 3
○ 4
○ m
○ p4

No, the answer is incorrect.
Score: 0

Accepted Answers:
4

17) The Hermann-Maugin symbols for the point groups for the pattern (Fig.below) is ________ *2 points*

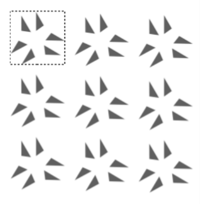


○ pm
○ 4m
○ p4m
○ m4

No, the answer is incorrect.
Score: 0

Accepted Answers:
4m

Carefully study the pattern in the figure and answer the following questions.



18) The motif indicated by the dashed box has *2 points*

○ three mirror planes
○ one 6 fold rotation axis
○ Two mirror planes
○ One four fold axis only

No, the answer is incorrect.
Score: 0

Accepted Answers:
three mirror planes

19) The point group of the motif indicated by the dashed box is

2 points

○ 6m1 or 61m
○ 3m1 or 31m
○ 3m
○ 4m

No, the answer is incorrect.
Score: 0

Accepted Answers:
3m1 or 31m

20) The plane group of this pattern (if repeated infintiely in the 2 directions is)

4 points

○ p3m1
○ 1
○ p1
○ p3m

No, the answer is incorrect.
Score: 0

Accepted Answers:
p1

Consider a crystal belonging to the space group $P4_2$,

21) The point group is ______

No, the answer is incorrect.
Score: 0

Accepted Answers:
(Type: Numeric) 4

1 point

22) The crystal system we can use to construct the crystal is

2 points

○ cubic
○ Tetragonal
○ rhombhohedral
○ square mesh in 2D

No, the answer is incorrect.
Score: 0

Accepted Answers:
Tetragonal

23) An atom is present at the fractional coordinate x, y, z. The multiplicity of this point _______

No, the answer is incorrect.
Score: 0

Accepted Answers:
(Type: Numeric) 4

6 points

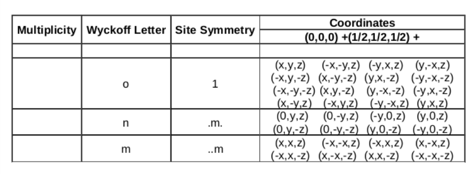
24) If the space group was $P4_2/m$ the multiplicity of a general point x, y, z ______

No, the answer is incorrect.
Score: 0

Accepted Answers:
(Type: Numeric) 8

6 points

The Table below shows the some positions of space group I4 $/mmm$. Carefully study the table and answer the following questions



Multiplicity	Wyckoff Letter	Site Symmetry	Coordinates (0,0,0) +(1/2,1/2,1/2) +
	o	1	(x,y,z) (-x,-y,z) (-y,x,z) (y,-x,z) (-x,y,-z) (x,-y,-z) (y,x,-z) (-y,-x,-z) (-x,-y,-z) (x,y,-z) (y,-x,-z) (-y,x,-z) (x,-y,z) (-x,y,z) (-y,-x,z) (y,x,z)
	n	.m.	(0,y,z) (0,-y,z) (-y,0,z) (y,0,z) (0,y,-z) (0,-y,-z) (y,0,-z) (-y,0,-z)
	m	..m	(x,x,z) (-x,-x,z) (-x,x,z) (x,-x,z) (-x,x,-z) (x,-x,-z) (x,x,-z) (-x,-x,-z)

25) This crystal can be constructed using a ________ unit cell

2 points

○ Cubic
○ Tetragonal

○ hexagonal
○ orthorhombic

No, the answer is incorrect.
Score: 0

Accepted Answers:
Tetragonal

26) If there is an atom at (0,0.35,0.22), then it is likely to be in Wyckoff position **3 points**

○ n
○ m
○ O
○ either o or m

No, the answer is incorrect.
Score: 0

Accepted Answers:
n

27) The multiplicity of position o is **3 points**

○ 32
○ 16
○ 4
○ 2

No, the answer is incorrect.
Score: 0

Accepted Answers:
32

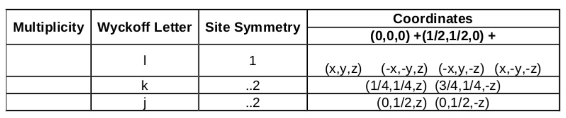
28) The point with fractional coordinates (0.9,0.8,0.6) generates another point inside the unit cell which is (______ , ______ , ______) **2 points**

○ (0.4,0.3,0.1)
○ (1.5,1.3,1.1)
○ (- 0.9,- 0.8,0)
○ (0.9,0.9,0.4)

No, the answer is incorrect.
Score: 0

Accepted Answers:
(0.4,0.3,0.1)

The Table below shows the some positions of space group C222. Carefully study the table and answer the following questions



Multiplicity	Wyckoff Letter	Site Symmetry	Coordinates
			(0,0,0) +(1/2,1/2,0) +
	l	1	(x,y,z) (-x,-y,z) (-x,y,-z) (x,-y,-z)
	k	..2	(1/4,1/4,z) (3/4,1/4,-z)
	j	..2	(0,1/2,z) (0,1/2,-z)

29) This crystal can be constructed using a ______ unit cell **2 points**

○ Cubic
○ Tetragonal
○ hexagonal
○ orthorhombic

No, the answer is incorrect.
Score: 0

Accepted Answers:
orthorhombic

30) If there is an atom at (0.44,0.35,0.22), then it is likely to be in Wyckoff position ______ **3 points**

○ l
○ k
○ j
○ either k or j

No, the answer is incorrect.
Score: 0

Accepted Answers:
l

31) The multiplicity of position l is **3 points**

○ 32
○ 16
○ 4
○ 8

No, the answer is incorrect.
Score: 0

Accepted Answers:
8

32) The point with fractional coordinates (0.9,0.8,0.6) generates another point inside the unit cell which is (_____ , _____ , _____) **2 points**

○ (-0.4,0.3,0.6)
○ (0.4,0.3,0.6)
○ (-0.4,0.3,-0.6)
○ (0,1/2,0.6)

No, the answer is incorrect.
Score: 0

Accepted Answers:
(0.4,0.3,0.6)

The Table below shows the some positions of space group $P3_221$. Carefully study the table and answer the following questions

Multiplicity	Wyckoff Letter	Site Symmetry	Coordinates
	c	1	(x,y,z) (-y,x-y,z+2/3) (-x+y,-x,z+1/3) (y,x,-z) (x-y,-y,-z+1/3) (-x,-x+y,-z+2/3)
	b	.2.	(x,0,1/6) (0,x,5/6) (-x,-x,1/2)
	a	.2.	(x,0,2/3) (0,x,1/3) (-x,-x,0)

33) This crystal can be constructed using a _____ unit cell *2 points*

○ Cubic
○ Tetragonal
○ Hexagonal
○ orthorhombic

No, the answer is incorrect.
Score: 0

Accepted Answers:
Hexagonal

34) If there is an atom at (0.44,0.35,0.22), then it is likely to be in Wyckoff position *3 points*

○ c
○ b
○ a
○ either b or a

No, the answer is incorrect.
Score: 0

Accepted Answers:
c

35) The multiplicity of position b is *3 points*

○ 4
○ 6
○ 3
○ 7

No, the answer is incorrect.
Score: 0

Accepted Answers:
3

36) The point with fractional coordinates (0.9,0.8,0.6) generates another point inside the unit cell which is (_____ , _____ , _____) *2 points*

○ (0.8,0.9,0.6)
○ (0.1,0.1,0.266666)
○ (0.9,0.8,1/6)
○ (1/6,0.8,0.9)

No, the answer is incorrect.
Score: 0

Accepted Answers:
(0.1,0.1,0.266666)

$CaMgSi_2O_6$ belongs to the space group $C1\frac{2}{c}1$. Given $a = 0.95848$, $b = 0.86365\ nm\ and\ c\ = 0.51355nm$ and the following table(Table 1), answer the following questions

Table 1: Positions of Ca, Mg, Si and O atoms

Atom	Wyckoff position	x	y	z
Ca1	4e	0	0.3069	0.25
Mg1	4e	0	0.9065	0.25
Si1	8f	0.284	0.0983	0.2317
O1	8f	0.1135	0.0962	0.1426
O1	8f	0.3594	0.2558	0.3297
O1	8f	0.3571	0.0175	0.9982

37) The C refers to *2 points*

○ A C centered lattice

○ A c glide
○ A Face centerd lattice
○ none of the above

No, the answer is incorrect.
Score: 0

Accepted Answers:
A C centered lattice

38) The multiplicity of Si1 atoms is ***2 points***

○ 4
○ 8
○ 8+4=12
○ 8-4=4

No, the answer is incorrect.
Score: 0

Accepted Answers:
8

39) I will use a _______ unit cell to construct this crystal ***2 points***

○ cubic
○ Orthorhombic
○ Tetragonal
○ Monoclinic

No, the answer is incorrect.
Score: 0

Accepted Answers:
Orthorhombic

40) The total number of single particle possible states ($\Phi_{<E^*}$)less than a given energy E^* ***3 points***

$$\Phi_{<\,E^*} = \frac{\pi}{6}\left(\frac{E^* 8mV^{\frac{2}{3}}}{h^2}\right)^{\frac{3}{2}}$$

If the temperature is 500K and the particle is confined to a volume of $1m^3$ the best approximation to the value of $\Phi_{<\,E^*}$ is

($Assume\ \ m = 10^{-23}kg,\ \ h = 6.62607004 \times 10^{-34} m^2 kgs^{-1}$ and $K_B = 1.38064852 \times 10^{-23} m^2 kgs^{-2} K^{-1}$)

○
10^{36}
○ 34
○
10^{4}
○ 10100

No, the answer is incorrect.
Score: 0

Accepted Answers:
10^{36}

41) For a double pendulum with degrees of freedom θ_1 and θ_2 , the kinetic T and the potential energies (V) are given by the following expressions ***5 points***

$$T = \frac{1}{2} m_1 l_1 \dot{\theta}_1^2 + \frac{1}{2} m_2 (l_1^2 \dot{\theta}_1^2 + l_2^2 \dot{\theta}_2^2 + 2 l_1 l_2 \dot{\theta}_1 \dot{\theta}_2 cos(\theta_1 - \theta_2))$$

$$V = -(m_1 + m_2) g l_1 cos(\theta_1) - m_2 g l_2 cos(\theta_2)$$

The Euler-Lagrange equations for θ_1 *are*

○
$(m_1 + m_2) l_1 \ddot{\theta}_1 + m_2 \ddot{\theta}_2 l_2 cos(\theta_1 - \theta_2) + m_2 l_2 \dot{\theta}_2^2 sin(\theta_1 - \theta_2) + g(m_1 + m_2) sin(\theta_1) = 0$
○
$m_2 l_2 \ddot{\theta}_2 + m_2 l_1 \ddot{\theta}_1 cos(\theta_1 - \theta_2) - m_2 l_1 \dot{\theta}_1^2 sin(\theta_1 - \theta_2) + m_2 g\ sin(\theta_2) = 0$
○
$m_1 l_2 \ddot{\theta}_2 + m_2 l_2 \ddot{\theta}_1 cos(\theta_1 - \theta_2) - m_2 l_1 \dot{\theta}_1^2 sin(\theta_1 - \theta_2) + m_2 g\ sin(\theta_2) = 0$
○
$(m_1 + m_2) l_2 \ddot{\theta}_1 + m_2 \ddot{\theta}_2 l_1 cos(\theta_1 - \theta_2) + m_2 l_2 \dot{\theta}_2^2 sin(\theta_1 - \theta_2) + g(m_1 + m_2) sin(\theta_2) = 0$

No, the answer is incorrect.
Score: 0

Accepted Answers:
$(m_1 + m_2) l_1 \ddot{\theta}_1 + m_2 \ddot{\theta}_2 l_2 cos(\theta_1 - \theta_2) + m_2 l_2 \dot{\theta}_2^2 sin(\theta_1 - \theta_2) + g(m_1 + m_2) sin(\theta_1) = 0$

42) In Statistical Mechanics, we need to solve Newton's equations of motion of nealy one mole of particle ***2 points***

○ True
○ False

No, the answer is incorrect.
Score: 0

Accepted Answers:
False

43) In phase space each point switches from one point to the otheraccording to Newton's equations of motion. Since all points correspond to the same macrostate, any property (other than the ones specified) change with time even at equilibrium ***2 points***

○ True

○ False

No, the answer is incorrect.
Score: 0

Accepted Answers:
True

44) If ρ is the density of points in phase space, p_i and q_i $(i, j = 1, 2, 3 \ldots N)$ are the momenta and position degrees of freedom, then the equation ***3 points***

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \sum_{i=1}^{N} \left[\frac{\partial \rho}{\partial q_i} \dot{q}_i + \frac{\partial \rho}{\partial p_i} \dot{p}_i \right] = 0$$

○ is always true

○ is true only at equilibrium

○ never true

○ only applicable for NVE ensemble

No, the answer is incorrect.
Score: 0

Accepted Answers:
is always true

45) The total number of classical microstates for a system is ***3 points***

$$\Omega = \frac{\omega}{N! h^{3N}}$$

which of the following is True

○ N ! in the equation is true only for NVE ensemble

○ This expression is true for when particles are indistinguishable

○ Since h occurs in the equation, this expression is true only for quntum systems and never for classical systems

○ None of the above

No, the answer is incorrect.
Score: 0

Accepted Answers:
This expression is true for when particles are indistinguishable

46) There are $\mathcal{N}$ systems and f energy levels. The number of ways we can have a certain distribution such that $a_1, a_2, a_3 \ldots\ldots a_f$ with energies energies $E_1, E_2, E_3, E_4 \ldots\ldots E_f$ is ***3 points***

○ $\dfrac{f!}{a_1!a_2!a_3!a_4!\ldots\ldots\ldots\ldots a_f!}$

○ $\dfrac{\mathcal{N}!}{a_1!a_2!a_3!a_4!\ldots\ldots\ldots\ldots a_f!}$

○ $\dfrac{f!}{a_1!a_2!a_3!a_4!\ldots\ldots\ldots\ldots a_f!} \times \dfrac{\mathcal{N}! + f!}{a_1!a_2!a_3!a_4!\ldots\ldots\ldots\ldots a_f!}$

○ $\dfrac{f!}{a_1!a_2!a_3!a_4!\ldots\ldots\ldots\ldots a_f!} + \dfrac{\mathcal{N}! + f!}{a_1!a_2!a_3!a_4!\ldots\ldots\ldots\ldots a_f!}$

No, the answer is incorrect.
Score: 0

Accepted Answers:

$$\frac{\mathcal{N}!}{a_1!a_2!a_3!a_4!\ldots\ldots\ldots\ldots a_f!}$$

47) If the Helmholtz free energy is ***3 points***

$$A \approx N k_b T \left[ln\left(\frac{N}{V} \left(\frac{h^2}{2\pi m k_B T} \right)^{\frac{3}{2}} \right) - 1 \right]$$

the chemical potential is

○ $k_b T ln\left(\dfrac{N}{V} \left(\dfrac{h^2}{2\pi m k_B T} \right)^{\frac{3}{2}} \right)$

○ $\dfrac{N k_B T}{V}$

○ $N k_B \left(ln\left(\dfrac{V}{N} \left(\dfrac{2\pi m k_B T}{h^2} \right)^{\frac{3}{2}} \right) + \dfrac{5}{2} \right.$

○ $k_b T ln\left(\dfrac{N}{V} \left(\dfrac{h}{\sqrt{2\pi m k_B T}} \right)^{\frac{3}{2}} \right)$

No, the answer is incorrect.
Score: 0

Accepted Answers:

$$k_bTln\left(\frac{N}{V}\left(\frac{h^2}{2\pi mk_BT}\right)^{\frac{3}{2}}\right)$$

48) The following two sequence of commands (Sequence1 and Sequence2) in a LAMMPS input script are the same *3 points*

Listing 1: Sequence 1

```
timestep 0.5
run      100
run 100
```

Listing 2: Sequence 2

```
run 100
timestep 0.5
run      100
```

○ True
○ False

No, the answer is incorrect.
Score: 0

Accepted Answers:
False

49) The basis fractional coordinates are specified in the ______ command *2 points*

○ create_box
○ region
○ lattice
○ dump

No, the answer is incorrect.
Score: 0

Accepted Answers:
lattice

50) For the run command, the number of steps can be specified by referring to a variable which was defined before in the input script *3 points*

○ True
○ False

No, the answer is incorrect.
Score: 0

Accepted Answers:
True

51) The units of pressure when the metal units are used is *2 points*

○ Pascals
○ bars
○ Mega Pascals for solids
○ Giga Pascals for solids

No, the answer is incorrect.
Score: 0

Accepted Answers:
bars

52) Which of the following pairs may be appropriate for the blanks provided for the following command in a LAMMPS input script is *3 points*

```
velocity 23 create _______ 103422 dist ________
```

○ uniform,45
○ 300,uniform
○ 25K, 30Pa
○ velocity,manual

No, the answer is incorrect.
Score: 0

Accepted Answers:
300,uniform

53) Which of the following best describes the role of the command *3 points*

```
minimize 1.0e-4 1.0e-6 100 1000
```

○ Calculate the minimum energy
○ A energy minimization
○ Reduce only forces to a finite value
○ Adjust the minimum time steps

No, the answer is incorrect.
Score: 0

Accepted Answers:
A energy minimization

54) Which of the following commands will stop printing out per-atom information? *2 points*

○ unfix
○ undump
○ print stop
○ stop print

No, the answer is incorrect.
Score: 0

Accepted Answers:
undump

55) A fix command must always be followed by a unfix command **3 points**

○ True
○ False

No, the answer is incorrect.
Score: 0

Accepted Answers:
False

56) The fix ave/time command is useful to average **3 points**

○ per atom quantities
○ global quantities
○ any atom position
○ anytime dependent quantity

No, the answer is incorrect.
Score: 0

Accepted Answers:
global quantities

57) The command `variable b equal ${v_temp}*Kb` is ____ **2 points**

○ Correct
○ Wrong
○ Correct if Kb is defined before in the input script
○ Correct if temp is calculate before in the input script

No, the answer is incorrect.
Score: 0

Accepted Answers:
Wrong

58) Periodic boundary conditions are used to calculate ______ properties of materials **2 points**

○ bulk
○ surface
○ average thermodynamics
○ simplied mechanical

No, the answer is incorrect.
Score: 0

Accepted Answers:
bulk

59) Which of the following properties can be determined using molecular dynamics? **2 points**

○ Electronic conductivity
○ Elastic stiffness tensor
○ Magnetic moments
○ Charges around atomic defects

No, the answer is incorrect.
Score: 0

Accepted Answers:
Elastic stiffness tensor

60) The specification of the following two commands are the same for all practical purposes **3 points**

Command 1:

```
region          myreg block     0 10 &
                                0 10 &
                                0 10 units box
```

Command 2 :

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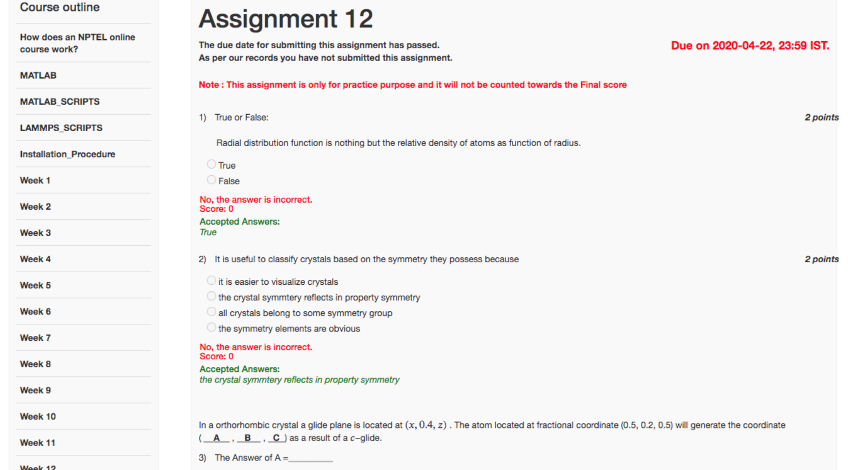

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How does an NPTEL online course work?

MATLAB

MATLAB_SCRIPTS

LAMMPS_SCRIPTS

Installation_Procedure

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Week 12

Assignment 12

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

Due on 2020-04-22, 23:59 IST.

Note : This assignment is only for practice purpose and it will not be counted towards the Final score

1) True or False: ***2 points***

Radial distribution function is nothing but the relative density of atoms as function of radius.

○ True
○ False

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

2) It is useful to classify crystals based on the symmetry they possess because ***2 points***

○ it is easier to visualize crystals
○ the crystal symmtery reflects in property symmetry
○ all crystals belong to some symmetry group
○ the symmetry elements are obvious

No, the answer is incorrect.
Score: 0
Accepted Answers:
the crystal symmtery reflects in property symmetry

In a orthorhombic crystal a glide plane is located at $(x, 0.4, z)$. The atom located at fractional coordinate (0.5, 0.2, 0.5) will generate the coordinate (__A__ , __B__ , __C__) as a result of a c–glide.

3) The Answer of A =__________