**Progress** 

Course outline

MATLAB\_SCRIPTS

LAMMPS\_SCRIPTS

Installation\_Procedure

Generation of monoclinic

Introduction to Statistical

Introduction to Statistical

Week 5 Lecture materials

Foundations of Computational

Ouiz: Assignment 5

Materials Modelling

Week 6

Week 7

Week 8

Week 9

Week 10

Week 11

Week 12

**Additional Documents** 

Download videos

**Text Transcripts** 

Week 5 Feedback :

course work?

MATLAB

Week 1

Week 2

Week 3

Week 4

Week 5

lattice

Mechanica 1

Mechanica 2

NPTEL » Foundations of Computational Materials Modelling

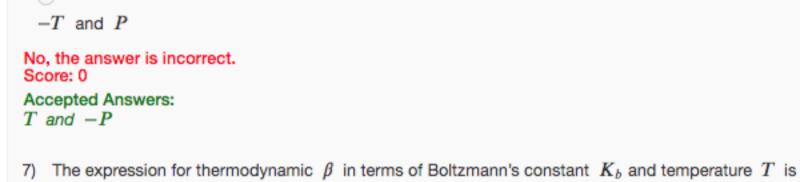
2 points

2 points

## Unit 10 - Week 5

How does an NPTEL online

	due date for submitting this assignment has passed.  Due on 2020-03-04, 23:  Due on 2020-03-04, 23:  Due on 2020-03-04, 23:  Due on 2020-03-04, 23:
1)	The sum of all the microscopic form of energy is called
	Total energy
	Phase energy
	System energy
	Internal energy
No,	the answer is incorrect. re: 0
Acc	epted Answers: rnal energy
2)	Statistical thermodynamics assumes the existence of atoms and molecules and provides explicit expressions for the macroscopic thermodynamic quantities which are used to calculate the quantity of interest in molecular dynamics
C	True
C	False
No,	the answer is incorrect.
Sco	re: 0 epted Answers:
True	
3)	Wyckoff position is a point belonging to a set of points for which site symmetry groups are conjugate subgroups of the space group
	True
	False
No,	the answer is incorrect.
	re: 0 epted Answers:
True	
4)	An isolated system having a constant number N of atoms occupying a volume V and a constant energy is called the microcanonical ensemble.
	True False
Sco	the answer is incorrect. re: 0
Acc True	epted Answers:
7740	
5)	The equation relating the entropy $S$ to the quantity $\Omega$ , the number of real microstates (corrsponding to a given macrostate) is
	$= k_B lnS$
	1
S	$=rac{1}{k_B}ln\Omega$
	$=k_Bln\Omega$
Ω	$=\frac{1}{k_B}lnS$
No,	the answer is incorrect. re: 0
Acc	epted Answers:
S' =	$k_B ln\Omega$
6)	Complete the following equations:
	$\langle \partial U \rangle$
	$\left(\frac{\partial \mathcal{C}}{\partial \mathcal{S}}\right)_{V,N} = \underline{\hspace{1cm}}$
	$\left(\frac{\partial U}{\partial V}\right)_{SN}^{V,N} = \underline{\hspace{1cm}}$
	$\left(\frac{\partial V}{\partial V}\right)_{S,N} =$



 $\overline{K_bT}$  $K_bT$  $\frac{K_b}{T}$ 

T $\overline{K_b}$ No, the answer is incorrect. Score: 0 Accepted Answers:  $\overline{K_bT}$ 

Accepted Answers:

 $\boldsymbol{P}$  and  $\boldsymbol{T}$ 

8) Classical or Newtonian mechanics generally deals with the connections between the microscopic degrees of freedom and macroscopic

False

thermodynamic properties ○ True False No, the answer is incorrect. Score: 0

9) A crystal belongs to the space group  $P4_1$  with a=b=0.9046nm and c=1.6714nm. One of the atoms is in the Wyckoff position 4a3 points with fractional coordinates 0.4169, 0.7330, 0.8359. The actual cartesian coordinates of this atom to two decimal places are X, and Z The values of x, y and z are:

x=1.39, y= 0.66 and z=0.38 No, the answer is incorrect. Score: 0 Accepted Answers:

x=0.38, y= 0.66 and z=1.39

x=1.40, y=0.28 and z= 0.36

x=0.38, y=1.39 and z= 0.66

x=0.38, y= 0.66 and z=1.39