

Unit 10 - Week 5

Course outline

How does an NPTEL online course work?

MATLAB

MATLAB_SCRIPTS

LAMMPS_SCRIPTS

Installation_Procedure

Week 1

Week 2

Week 3

Week 4

Week 5

Generation of monoclinic lattice

Introduction to Statistical Mechanics 1

Introduction to Statistical Mechanics 2

Week 5 Lecture materials

Quiz : Assignment 5

Week 5 Feedback : Foundations of Computational Materials Modelling

Week 6

Week 7

Week 8

Week 9

Week 10

Week 11

Week 12

Additional Documents

Download videos

Text Transcripts

Assignment 5

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

Due on 2020-03-04, 23:59 IST.

1) The sum of all the microscopic form of energy is called 2 points

- Total energy
 Phase energy
 System energy
 Internal energy

No, the answer is incorrect. Score: 0

Accepted Answers: Internal 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 2 points

- True
 False

No, the answer is incorrect. Score: 0

Accepted 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 2 points

- True
 False

No, the answer is incorrect. Score: 0

Accepted 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. 2 points

- True
 False

No, the answer is incorrect. Score: 0

Accepted Answers: True

5) The equation relating the entropy S to the quantity Ω , the number of real microstates (corrsponding to a given macrostate) is 2 points

- $\Omega = k_B \ln S$
 $S = \frac{1}{k_B} \ln \Omega$
 $S = k_B \ln \Omega$
 $\Omega = \frac{1}{k_B} \ln S$

No, the answer is incorrect. Score: 0

Accepted Answers: $S = k_B \ln \Omega$

6) Complete the following equations: 2 points

$$\left(\frac{\partial U}{\partial S}\right)_{V,N} = \underline{\hspace{2cm}}$$

$$\left(\frac{\partial U}{\partial V}\right)_{S,N} = \underline{\hspace{2cm}}$$

- $-P$ and $-T$
 T and $-P$
 P and T
 $-T$ and P

No, the answer is incorrect. Score: 0

Accepted Answers: T and $-P$

7) The expression for thermodynamic β in terms of Boltzmann's constant K_b and temperature T is 2 points

- $\frac{1}{K_b T}$
 $K_b T$
 $\frac{K_b}{T}$
 $\frac{T}{K_b}$

No, the answer is incorrect. Score: 0

Accepted Answers: $\frac{1}{K_b T}$

8) Classical or Newtonian mechanics generally deals with the connections between the microscopic degrees of freedom and macroscopic thermodynamic properties 2 points

- True
 False

No, the answer is incorrect. Score: 0

Accepted Answers: False

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 $4a$ with fractional coordinates 0.4169, 0.7330, 0.8359. The actual cartesian coordinates of this atom to two decimal places are X , Y and Z 3 points

The values of x, y and z are:

- $x=1.40, y=0.28$ and $z= 0.36$
 $x=0.38, y=1.39$ and $z= 0.66$
 $x=0.38, y= 0.66$ and $z=1.39$
 $x=1.39, y= 0.66$ and $z=0.38$

No, the answer is incorrect. Score: 0

Accepted Answers: $x=0.38, y= 0.66$ and $z=1.39$