

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -3 EXAMINATION- 2023

B.Tech-VII Semester (CSE/IT/ECE/CE/BT/BI)

COURSE CODE (CREDITS): 22B1WPH731 (3)

MAX. MARKS: 35

COURSE NAME: Computational Nanotechnology

COURSE INSTRUCTORS: Dr. Santu Baidya

MAX. TIME: 2 Hours

*Note: (a) All questions are compulsory.*

*(b) Marks are indicated against each question in square brackets.*

*(c) The candidate is allowed to make Suitable numeric assumptions wherever required for solving problems*

Q1. What is a primitive unit cell and non-primitive unit cell? Write down the primitive lattice parameters of a face-centered cubic cell. [CO-3] [2+3]

Q2. A ball at 1200 K temperature is allowed to cool down in air at an ambient temperature of 300 K. Assuming heat is lost only due to radiation, the differential equation for the temperature of the ball is given by

$$\frac{d\theta}{dt} = -2.2067 \times 10^{-12} (\theta^4 - 81 \times 10^8), \theta(0) = 1200 K$$

Where  $\theta$  is in Kelvin and  $t$  is in second. Find the temperature at  $t = 480$  second using Runge-Kutta 4<sup>th</sup> order method. [CO-2] [5]

Q3. Write down the basic assumptions of the Thomas-Fermi approximation for many-electron system. Write down the Thomas-Fermi energy functional  $E_{TF}[\rho]$  as a function of electron density of an atom. [CO-5] [3+2]

Q4. What are the statements of the Hohenberg-Kohn theorem? Prove the two statements. [CO-5] [2+3]

Q5. What is local density approximation (LDA)? What is the form of exchange-correlation energy functional under LDA for without spin and with spin system? [CO-1] [1+4]

Q6. What is Kohn-Sham approximation for solving many-electron system? Write down the energy functional given by Kohn-Sham approximation. What is the formula for exchange-correlation energy functional? [CO-3] [2+4+4]