

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -1 EXAMINATION- 2023

B.Tech-7 Semester (CSE/IT/ECE/CE)

COURSE CODE(CREDITS): 3

MAX. MARKS: 15

COURSE NAME: Computational Nanotechnology (22BIWPH731)

COURSE INSTRUCTORS: Dr. Santu Baidya

MAX. TIME: 1 Hour

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. Write briefly on how do the size affect properties of Nanomaterials. Explain the two most important size dependent effects due to which properties changes on reduction of dimension.

[1+2]

Q2. Define electronic density of states (DOS) and write down the expression for 2D DOS. Plot the DOS for 3D, 2D, 1D and 0D.

[1+2]

Q3. Calculate the number of available density of states per unit volume of a bulk Si between 0 eV and 1 eV energy window.

[3]

Q4. Define a Bravais lattice and give an example of a non-Bravais lattice with sketch. What is van Hove singularity?

[2+1]

Q5. Find $y(0.1)$ for $y'' = 1 + 2xy - x^2z$ with initial conditions $x_0 = 0, y_0 = 1$ and $z_0 = 0$ with $h=0.1$ using Runge-Kutta 4th order method.

[3]