

JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

TEST -1 EXAMINATION- 2024

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

COURSE CODE(CREDITS): 22B1WPH731 (3)

MAX. MARKS: 15

COURSE NAME: Computational Nanotechnology

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. Explain the classifications of nanomaterials in terms of their sizes and give examples of real materials for each type. [3]

Q2. Explain what are the two important reasons to see strange properties in nanomaterials (explain with details). How does electronic properties changes going to nano-dimension (explain) [2+1]

Q3. Define Bravais lattice. Is graphene a Bravais lattice (explain)? How does one convert a non-primitive unit cell into a primitive unit cell? [1+2+1]

Q4. A Bravais lattice is specified by the primitive lattice vectors:

$$\vec{a}_1 = a \hat{x}, \vec{a}_2 = \frac{1}{2} a \hat{x} + \frac{\sqrt{3}}{2} a \hat{y}, \vec{a}_3 = c \hat{z}$$

Where \hat{x} , \hat{y} , and \hat{z} are the unit vectors along the x, y, and z directions respectively, and a is the lattice constant. We assume that $c > 2a$. Find the Reciprocal lattice vectors of the given lattice.

[3]

Q5. Define electronic density of states. Draw figures for 0, 1, 2, and 3 dimensional density of states for nanomaterials. [1+1]