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

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Q1. Write down the statements of Hohenberg-Kohn theorem. Explain how does density functional theory differs from Hartree-Fock method? **[CO-3] [4+2]**

Q2. Write down the total energy functional obtained from Kohn-Sham density functional approximation. Explain each term. **[CO-3] [5]**

Q3. What is exchange-correlation energy functional in density functional theory? Can you write down the analytical form of the exchange functional part? **[CO-5] [3+3]**

Q4. Use the DFT software TB-LMTO-ASA to calculate the band structure for the bulk Ge, whose atomic positions and lattice parameters are given below. For calculation, choose LDA exchange-correlation functional option in the code. Take snapshot picture to prove that you got self-consistency (Jolly Good Show!) after lm.run. Also, write the band gap obtained from total band structure for Ge and write the error in the DFT calculation (Original band gap of Ge ~ 0.67eV). Save in the ps format with the name of file such as "Roll-number-band-Ge.ps"

Bulk Ge

Space group: Fd-3m (227); a=b=c=5.67 Å, Ge: x=0.00 y=0.00 z=0.50 (atomic position)

(Put the output files in the folder \\172.16.73.6\Physics\Faculty\Computational Nanotechnology T3 Lab) **[CO-2] [8+6+4]**