JAYPEE UNIVERSITY OF INFORMATION TECHNOLOGY, WAKNAGHAT

Comprehensive Examination - 2025

Ph.D (PMS)

COURSE CODE (CREDITS): 17P1WPH131 MAX. MARKS: 100

COURSE NAME: Comprehensive test

COURSE INSTRUCTORS: SBA MAX. TIME: 3 Hours

Note: (a) All questions are compulsory.

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

Sec A

Q.No	Question	Marks
Q1	(a) What are the factors on which the adsorption of a gas molecules depend on? Explain each point. (b) Define molecule adsorption energy with equation and explain each term. (c) What is physisorption and chemisorption? Explain very well.	10 4 6
Q2	(a) What is exchange interactions in a magnetic solid? Write down the Heisenberg Hamiltonian for ferromagnetic exchange interaction between two types of magnetic atoms A and B arranged in one dimension and explain it. (b) What is quantum anomalous Hall effect? Explain with diagram.	2+6 6

Sec B

Q.No	Question	Marks
Q3	(a) Define reciprocal lattice and explain the construction of primitive unit cell in the reciprocal lattice. (b) Show that the reciprocal lattice of a bcc lattice is a fcc lattice.	4 4
Q4	(a) Derive Bragg's law of X-ray diffraction on a crystal. (b) What are Miller indices? Obtain the Miller indices of planes having intercepts (a, b/2, 3c) in SC structure.	6 2+4
Q5	(a) Explain the Kronig-Penny model and explain band gap. (b) Draw the plots for the variation of the resistivity with temperature for a semiconductor and a metal. Explain both the plots.	8 2
Q6	(a) Define phonons in a crystal. Explain the properties of two types of phonons comparatively.	1+2

Sec C

Q.No	Question	Marks
Q7	(a) Explain the Born-Oppenheimer approximation and why is it called adiabatic approximation? (b) Write down the total Hamiltonian of an N_e electron and NA atoms solid and explain each term in the Hamiltonian. (c) Use Born-Oppenheimer approximation to the total Hamiltonian and write the Hamiltonian for electrons only.	1+1 2 2
Q8	(a) What was the failure of Born-Oppenheimer approximation to lead to Hartree approximation? (b) What is Hartree approximation? Explain very well. (c) Describe Hartree-Fock approximation.	3 2 3
Q9	(a) Prove that the Slater determinant supports Pauli exclusion principle. (b) Write down the integral form of exchange integral and Coulomb integral obtained from Hartree-Fock theory.	3 3
Q10	(a) Write down the Hohenberg-Kohn theorem and prove them. (b) Define basis function and how can a total wave function of a molecule be expressed in terms of basis functions?	6 2+5

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