FE Sem-II (NEP2020) May 2026

20/5/26

Time: 1 ½ hours **Max. Marks: 45**

N.B.:
(i) Question No.1. is compulsory.
(ii) Attempt any two questions out of remaining Four questions.
(iii) Assume suitable data and justify the same.
(iv) Figures to the right indicate full marks.

Q1	Solve any Five.	(15 Marks)
A	What are the features of Wave function?	
B	Explain why bonding is not possible in case of Be2 molecule?	
C	Give any 2 applications of computational chemistry.	
D	Explain Slater (STO) & Gaussian (GTO) type orbitals in Basis sets.	
E	Explain Born Oppenheimer approximation.	
F	Define Local, Global minima & Saddle point.	
G	Explain Electron density as a concept.	
Q2		(15 Marks)
A	Explain basics of Valence bond theory. What do you mean by stationary wave?	
B	An electron in H atom is moving with velocity of 5×10^{6} m/s.If the uncertainty in the momentum is 1.5%, calculate uncertainty in position of electron. ($m_{el} = 9.109 \times 10^{-31}$ kg, $h = 6.626 \times 10^{-34}$ Js)	
C	What is parameterisation & iteration in computational chemistry?	
Q3		(15 Marks)
A	Give the Principle of Density Field Theory & explain Hohenberg -Kohn theorems.	
B	What is the scope of Computational chemistry? Elaborate with **One** example.	
C	Explain: a) Spin orbital b). Slater determinant.	
Q4		(15 Marks)
A	What do you mean by Computational investigation?	
B	Explain Azimuthal & Magnetic quantum no. What is their significance?	
C	Using MOT, explain magnetic character of NO.	
Q5		(15 Marks)
A	Define Force fields. Give any 3 examples of it.	
B	What are Coulomb & exchange integrals? Where do you use them?	
C	Explain Molecular dynamics.	

****