(1) Propose a detailed stepwise protocol to calculate the free energy surface corresponding to the conformational change of n-butane solvated in methanol. (4)

(2) What is molecular mechanics? Write the potential energy equation and explain all terms. (5)

(3) What are the limitations of force field. (2)

(4) Given $\phi_1(1)$, $\phi_2(2)$ and $\phi_3(3)$ are three molecular orbitals of a given molecule, write the overall wave function of the molecule. (3)

(5) Variational method allows obtaining an approximate wave function of molecules after Born-Oppenheimer approximation. How does one identify the minima on the potential energy surface if the nuclei are fixed in the process. (3)

(6) Why a regular molecular dynamics simulation is inefficient for studying protein folding dynamics? Propose a method using which one can address this issue. Explain in detail. (4)

(7) Explain using a flowchart or pseudo-code (with relevant equations) a molecular dynamics simulation. (4)

(8) Explain mean field approximation, and its role in Hartree-Fock method. (3)

(9) Using Hückel molecular orbital method to explain the stabilization of 1,3-butadiene due to π-conjugation. (5)