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Thermodynamics of Hydration of Fullerols [$C_{60}(OH)_n$] and Hydrogen – Bond Dynamics in the Hydration Shells SONANKI KESHRI, BHALACHANDRA TEMBE, Indian Inst of Tech-Bombay — Molecular dynamics simulations of fullerene and the water soluble derivatives of fullerene i.e. fullerols [$C_{60}(OH)_n$, where n = 2 to 30] in aqueous solutions have been performed for the purpose of obtaining a detailed understanding of the structural and dynamic properties of these nanoparticles in water. The study is motivated by the diverse biological applications of water-soluble fullerols. From the analysis of radial distribution functions, we have found that water molecules form two solvation shells around the central solute molecule. Hydrogen bonding in the bulk solvent is unaffected by increasing n. There is a large increase in H-bonding between solute and solvent molecules as we increase n. The diffusion constants of solute molecules decrease with increasing n. The fullerene molecules are found to have a very high ΔG in water ($\Delta G = 52.8$ kJ/mol), whereas a very low ΔG of $C_{60}(OH)_{30}$ (ΔG = -427.1 kJ/mol) in water have been found. Our simulation results reveal that the hydrophobic character of fullerene is reduced with surface hydroxylation.

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