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Hydrophobic polymers in nano-sized water droplets BUDDHI TILAKARATNE, University of Houston, SAMINA MASOOD, University of Houston, Clear Lake, MARGARET CHEUNG, University of Houston — As simulations of biopolymers take place in confined and tight spaces, such as protein folding in the interior of bacteria chaperones or the exit tunnels of ribosomes, quantitative analyses of the confinement effects on both biopolymers and solvent molecules become the center of attention as the solvent-mediated interactions are too profound to solve analytically. We are in the progress to investigate the solvation of hexane molecules in various nano-sized water droplets. Free energy profiles for a single hexane molecule in droplets show that the droplet surfaces are favored. Averaged configurations of hexane molecules at the interior and the surface are computed using the umbrella sampling methods. The implications of our results for protein stability in confined spaces will be discussed.

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