SIMULATIONS AND SPECTROSCOPY: STUDYING PROTEIN ADSORPTION VIA SFG AND MD

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The behavior of adsorbed proteins and peptides at interfaces is important in the problem of biocompatibility. Polarization analysis of Sum Frequency Generation (SFG) vibrational spectra has been employed to study the adsorption of simple antimicrobial peptides such as magainin, melittin, and tachyplesin onto polymer thin films to yield orientational information. These results are then compared to a model peptide/polymer interface in atomistic molecular dynamics simulations to examine the effects of factors such as aggregation, surface hydrophobicity, and roughness on the orientation and conformation of model alpha helix and beta sheet peptides at interfaces. We apply the simulation results to gain a better understanding of adsorption at a molecular level.