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**Molecular dynamics simulations of peptides interacting with a surface: Do surfaces prevent or promote aggregation?** MIRIAM FRIEDEL, JOAN-EMMA SHEA, University of California, Santa Barbara — Understanding the process of protein and peptide aggregation is critical to treating and preventing debilitating diseases such as Alzheimer's. In particular, there is evidence that the aggregation process may be influenced by protein-surface or protein-membrane interactions. Nevertheless, there have been few molecular dynamics (MD) studies of proteins and peptides interacting with surfaces. Here, we present the results of an MD study of an off-lattice peptide model. Simulations of peptides both in a bulk environment and interacting with a hydrophobic surface were performed. With this simple model, we examined the impact of peptide sequence and surface hydrophobicity on the thermodynamics and kinetics of aggregation, and our results indicate that both play a significant role in determining aggregation behavior. Although interaction with a surface allows the peptides to form aggregates not easily achieved in the bulk, the kinetics of assembly is not necessarily enhanced by the presence of a surface.

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