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Surface Effects on the Dynamics of Confined Short Peptides: A Computational Study LUIS CRUZ, Drexel Univ — In the cell, proteins perform their biological function by folding into their native state within confined spaces naturally provided by membranes and chaperones, among others. Of particular importance are proteins that do not have a native state, known as intrinsically disordered proteins (IDP), that exist mainly in random structures whose function is not well understood. Some of these IDPs, known to misfold and aggregate, have been associated with neurological diseases, such as the amyloid beta-protein (Abeta) in Alzheimer's disease. Here, results derived from molecular dynamics simulations will be presented that highlight the effects of different surfaces of confining pores on the dynamics of two fragments of the full-length Abeta, the Abeta(21-30) and Abeta(16-22) peptides. Simulations reveal that confinement in these nanometer-sized pores significantly change the dynamics of the peptides, and in particular, can stabilize transient structures by affecting the solvent within these pores. The degree of stability of structure will be shown to involve the delicate role of the confined solvent on mediating the peptide-surface interactions. Possible connections with amyloid formation and aggregation will be discussed.

Luis Cruz Cruz
Drexel Univ

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