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Protein Unfolding and Alzheimer's

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Early interaction events of beta-amyloid ($A\beta$) proteins with neurons have been associated with the pathogenesis of Alzheimer's disease. Knowledge pertaining to the role of lipid molecules, particularly cholesterol, in modulating the single $A\beta$ interactions with neurons at the atomic length and picosecond time resolutions, remains unclear. In our research, we have used atomistic molecular dynamics simulations to explore early molecular events including protein insertion kinetics, protein unfolding, and protein-induced membrane disruption of $A\beta$ in lipid domains that mimic the nanoscopic raft and non-raft regions of the neural membrane. In this talk, I will summarize our current work on investigating the role of cholesterol in regulating the $A\beta$ interaction events with membranes at the molecular level. I will also explain how our results will provide new insights into understanding the pathogenesis of Alzheimer's disease associated with the $A\beta$ proteins.