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Binding of amyloid peptides to lipid bilayers: effects of ions and lipid content[1] YANXING YANG, SHARAREH JALALI, CRISTIANO.L DIAS, New Jersey Inst of Tech — In amyloid diseases, cell toxicity can emerge from interactions of peptides with the cell membrane. In particular, amyloid peptides can form pores in the cell membrane and/or induce lipid loss through a detergent-like mechanism. Several factors have been shown to modulate the magnitude of these peptides-bilayer interactions, which can enhance or inhibit cell toxicity. These factors include lipid composition and the presence of ions in the solution. Here, we perform all-atom molecular dynamics simulations to provide an understanding at the atomic level of peptide-bilayer interactions and their modulation by Ca and selected lipids. Simulations are performed using amphipathic sequences inspired by amyloid peptides and bilayers make from palmitoyloleoyl-phosphatidycholine lipids. We find that both electrostatic and hydrophobic interactions contribute to peptide-bilayer binding. Specifically, binding is initiated with positively charged residues interacting with lipid head groups. Hydrophobic interactions sustain this bound state. The latter accounts for an irreversible bound state at room temperature. I will discuss these mechanisms in detail as well as how they are affected by Ca and selected lipid content of the bilayer.

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