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Protein aggregation and self-assembly into amyloid-like fibrils[1]
SHARAREH JALALI, YANXING YANG, FARBOD MAHMOUDINOBAR, CRISTIANO L. DIAS, Department of Physics, New Jersey Institute of Tech — Protein-based hydrogels are emerging as important structures for the development of biomedical applications due to their biocompatibility and mechanical properties, which can be engineered by fine-tuning the self-assembly process of the constituent proteins. This process involves the formation of supramolecular structures from alpha-helical or beta-sheet peptides. An understanding of how these structures are formed at the atomic level remains poorly understood. Here, we use all atom molecular dynamics simulations in explicit solvent to investigate the self-assembly process of amphipathic peptides with alternating polar and non-polar residues that form amyloid-like fibril structures. Large size and long-time simulations (up to 10 us) are used for sequences varying in the degree of hydrophobicity of their non-polar residues. We report on the effect of temperature and salt-content on fibril formation. In particular, we highlight the important role of hydrophobicity by showing that increasing temperature accelerates and slows down fibril formation for sequences with high and low hydrophobic characters, respectively. We also show that NaCl can promote fibril formation.

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