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Role of mutation on fibril formation in small peptides by REMD

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Amyloid fibrils are now recognized as a common form of protein structure. They have wide implications for neurological diseases and entities involved in the survival of living organisms, e.g., silkmoth eggshells. Biological functions of these entities are often related to the superior mechanical strength of fibrils that persists over a broad range of chemical and thermal conditions desirable for various biotechnological applications, e.g., to encapsulate drugs. Mechanical properties of fibrils was shown to depend strongly on the amino acid sequence of its constituent peptides whereby bending rigidities can vary by two orders of magnitude. Therefore, the rational design of new fibril-prone peptides with tailored properties depends on our understanding of the relation between amino acid sequence and its propensity to fibrillize. In this presentation I will show results from extensive Replica Exchange Molecular Dynamics (REMD) simulations of a 12-residue peptide containing the fibril-prone motif KFFE and its mutants. Simulations are performed on monomers, dimers, and tetramers. I will discuss effects of side chain packing, hydrophobicity, charges and beta-sheet propensity on fibril formation.

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