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Difference in aggregation between functional and toxic amyloids studied by atomistic simulations MARTIN CARBALLO PACHECO, Research Center Juelich and RWTH Aachen University, AHMED E. ISMAIL, RWTH Aachen University, BIRGIT STRODEL, Research Center Juelich and Heinrich Heine University Duesseldorf — Amyloids are highly structured protein aggregates, normally associated with neurodegenerative diseases such as Alzheimer's disease. In recent years, a number of nontoxic amyloids with physiologically normal functions, called functional amyloids, have been found. It is known that soluble small oligomers are more toxic than large fibrils. Thus, we study with atomistic explicit-solvent molecular dynamics simulations the oligomer formation of the amyloid-β peptide Aβ_{25-35}, associated with Alzheimer's disease, and two functional amyloid-forming tachykinin peptides: kassinin and neuromedin K. Our simulations show that monomeric peptides in extended conformations aggregate faster than those in collapsed hairpin-like conformations. In addition, we observe faster aggregation by functional amyloids than toxic amyloids, which could explain their lack of toxicity.

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