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【901】Amyloid fibril growth: A multiscale view

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The accumulation of amyloid fibrils is the hallmark of Parkinson's and Alzheimer's disease. We use atomistic and coarse-grain simulations to explore the intricate dynamics and aggregation of α-synuclein and amyloid-β(42), the proteins associated with these disorders.
We represent α-synuclein as a chain of deformable particles that can adapt their geometry, binding affinities and rearranges into disordered and ordered structures. Results offer valuable insight into the internal dynamics of α-synuclein and indicate that a protein attaching to a fibril gets trapped in sub-optimal configurations, explaining the experimentally observed stop-and-go-growth of an amyloid fibril.
We use atomistic simulations to explore the peptide dissociation from an amyloid-β(42) fibril. Simulations show structural stability of the fibrillar core and high flexibility registered at the tip.

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