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"*Stability and self assembly mechanism of synthesized anti freeze peptides nanotubes using Transition Path Sampling*"

Abstract:

Anti-freeze proteins (AFPs) have a surprisingly strong effect on the freezing point of water [1,2] , lowering it much more (up to 500 times) than the colligative effect. AFPs have evolved in fish, insects, plants, fungi, bacteria and allow organisms to survive in polar areas. Moreover, these proteins have application in the food industry, for example by preventing recrystallisation in ice-cream. Complementing experimental efforts to construct self-assembling anti-freeze peptide nanotubes (AFPNTs) from synthetic cyclic peptides [3,4,5] incorporating the hyperactive motif [-THR-ALA-THR-], we address here the stability and self-assembly mechanism of AFPNTs using MD simulations and Transition Path Sampling [6]. The stability of AFPNTs increases with size, by increasing the intermolecular backbone hydrogen bonds between the stacked cyclic peptides. Analysis of transition path sampling simulations show three types of nanotube growth mechanisms: 1) docking of the peptide directly at end of the tube followed by a locking step through hydrogen bond formation, 2) docking of a peptide into a metastable state in which a side chain penetrates the hollow tube, followed by a locking step forming the proper backbone hydrogen bonds. 3) docking of the peptide on the side the tube, followed by sliding along the tube to the end, and finally forming backbone hydrogen bonds in a locking step. This finding has consequences for the growth kinetics of AFP nanotubes.

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