Recent advances in the simulation of protein folding transitions and mechanical polymer stretching.

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Abstract : I will discuss some of our recent results in the simulation and analysis of three types of single-molecule configurational transitions:
(a) The unfolding of anhydrous proteins and protein ions triggered by protonation and unhindered "tumbling" in a low-pressure inert gas,
(b) The nature of the spontaneous refolding transition of denatured proteins in the absence of water, and
(c) The mechanical (or "force-induced") stretching transition of various polymers, including polypeptides with variable primary sequences, as well as grafted polyethylene chains with nontrivial transient topologies.
All structural changes are discussed in terms of the evolution of chain compactness and chain entanglements. This approach allows us to understand the transitions as an interplay between the generic polymer collapse and the specific local features that depend on composition.

Some recent relevant references:

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