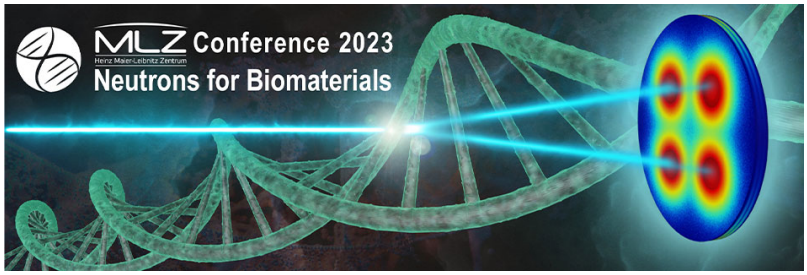

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Structure and dynamics during hydrophobic collapse of elastin-like polypeptides

Wednesday, May 24, 2023 10:40 AM (40 minutes)

Elastin-like polypeptides (ELPs) are versatile responsive biopolymers used in a range of biomedical applications such as drug delivery, protein purification and tissue engineering in the last decade. ELPs mimic a hydrophobic amino acid repeat segments of elastin which is a key protein of the extracellular matrix, and provides elastic properties to biological tissues –such as lung and ligaments –with extraordinary long-term stability and resilience. Elastin and ELPs undergo a hydrophobic collapse upon crossing a lower critical solution temperature (LCST), which can cause both compaction of individual chains, and the formation of ELP condensates. Although key to the elasticity of elastin and the stimulus-response of ELPs, a comprehensive mechanistic characterization of the collapse in terms of dynamical and structural evolution is so far missing. We report on an integrative research program combining dynamic and static scattering techniques with computer simulations. To study the interaction between amino acid segments, we first study a short ELP chain of 18 amino acids. From dynamic light scattering (DLS), we obtain a clear signature of chain assembly, which is also supported by an increasing size using small-angle neutron scattering (SANS). Computer simulation show that these short ELPs collapse only mildly, but show a temperature-induced attraction and form transient complexes [1]. Interestingly, the chains remain extended in simulations, while at the same time the complexes appear more compact after collapse based on the scattering signature. Finally, the chain dynamics explored by quasi-elastic neutron scattering (QENS) shows no strong dynamic transition, evidencing very dynamic, fluid-like assemblies.
Experimental signatures for longer ELP chains show a more diverse behavior with significant effects both on structure and dynamics as seen from QENS, SANS and DLS. Despite stronger chain collapse, we still obtain a high dynamic flexibility, rejecting earlier explanations for the hydrophobic collapse based on the formation of specific secondary structures. Finally, we use time-resolved small-angle X-ray scattering after a temperature jump induced by an IR laser to follow the millisecond structural evolution of hydrophobic collapse and formation of condensates, which shows a complex behavior.

[1] TI Morozova, NA García, O Matsarskaia, F Roosen-Runge, J-L Barrat: Structural and Dynamical Properties of Elastin-Like Peptides near Their Lower Critical Solution Temperature, Biomacromolecules 2023, in press, doi:10.1021/acs.biomac.3c00124

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