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Towards time-resolved protein dynamics on nanoscopic scales

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Protein function is realized by an interplay of molecular structure and dynamics. Although various methods have been established to study the evolution of macromolecular conformation after trigger events, the time-resolved evolution of protein dynamics on molecular length scales presents experimental challenges, in particular in the native environment in solution [1].

Here, we present a case study by quasi-elastic neutron scattering addressing the evolution of nanoscopic protein dynamics during thermal denaturation [2]. Using so-called elastic and inelastic fixed window scans, we obtain time-resolved information on the change of dynamics and the related dynamical confinement on nanometer length and nanosecond time scales. Upon heating, the dynamics first increase due to thermal activation, and then dramatically drop down upon unfolding and cross-linking. The slower dynamics is preserved when cooling back, due to the formed protein gels. The emerging picture thus includes a flexible motion of the protein network on nanosecond time scales, which is simply slowed down by the presence of the cross-linked neighbors.

The experimental approach allows to follow nanoscopic dynamics with a sampling time below one minute, which opens opportunities for dynamical changes e.g. driving protein assembly.

[1] M Grimaldo, F Roosen-Runge, F Zhang, F Schreiber, T Seydel, *Quart.Rev. Biophys.* 2019, 52, e7

[2] O Matsarskaia, L Bühl, C Beck, et al., *Phys.Chem.Chem.Phys.* 2020, 22, 18507-18517

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