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Conformational dynamics of proteins studied by time resolved small angle X-ray scattering combined with THz irradiation

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Conformational dynamics of proteins studied by time resolved small angle X-ray scattering combined with THz irradiation

Proteins rely on conformational changes to perform complex biochemical tasks. This dynamic plasticity can be modeled by large scale vibrational modes that have theoretical resonance frequencies in the range of 0.3 to 6 THz and can therefore be triggered by THz radiation. Since these modes are associated with conformational changes of several Angstrom to nm, they can be probed by small angle X-ray scattering (SAXS). We aim to observe synchronized collective vibrational modes in time resolved SAXS experiments with external THz excitation. Apart from standard protein samples, we aim to investigate porcine microtubules and human dipeptidyl peptidase 3 (DPP3). These systems exhibit large scale conformational plasticity and characeristic SAXS profiles.

The major challenge for this type of experiment is the sample environment. The harsh conditions under X-ray irradiation require constant material flow during the SAXS experiment. Simultaneous irradiation with THz radiations requires a thin liquid film ($< 200\mu$m) to compensate for the high absorption coefficient of aqueous solutions in the THz regime. Furthermore, window materials for X-ray and THz transmission have to be chosen with great care to avoid excess absorption or scattering artefacts. We design flow cells that fullfill these requirements to enable combined SAXS-THz experiments.

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