In this presentation, I will highlight research opportunities and challenges in probing structural dynamics of molecular systems using X-ray Photon Correlation Spectroscopy (XPCS). The development of new X-ray sources, such as 4th generation storage rings and X-ray free-electron lasers (XFELs), provides promising new insights into molecular motion. Employing XPCS at these sources allows to capture a very broad range of timescales and lengthscales, spanning from femtoseconds to minutes and atomic scales to the mesoscale. Here, I will discuss the scientific questions that can be addressed with these novel tools for two prominent examples: the dynamics of supercooled water [1,2] and proteins [3]. Finally, I will provide practical tips for designing and estimating feasibility of XPCS experiments as well as on detecting and mitigating radiation damage.

Figure 1. A typical experimental setup of X-ray Photon Correlation Spectroscopy (XPCS). The scattering intensity is recorded with a pixelated 2D array detector. The scattering intensity is recorded as a function of time, which fluctuates due the changes of the speckle pattern (upper right-hand panel). By calculating the intensity correlation function g2 one can obtain information about the dynamics. The amplitude of the correlation function relates to the speckle contrast β and the decay constant reflects the timescale of motion associated with the given momentum transfer Q.


Keywords: X-ray Photon Correlation Spectroscopy; XPCS; Supercooled Water; Protein dynamics