Molecular movies with X-ray photon correlation spectroscopy

F. Perakis

Physics Department, Stockholm University, Sweden

f.perakis@fysik.su.se

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.

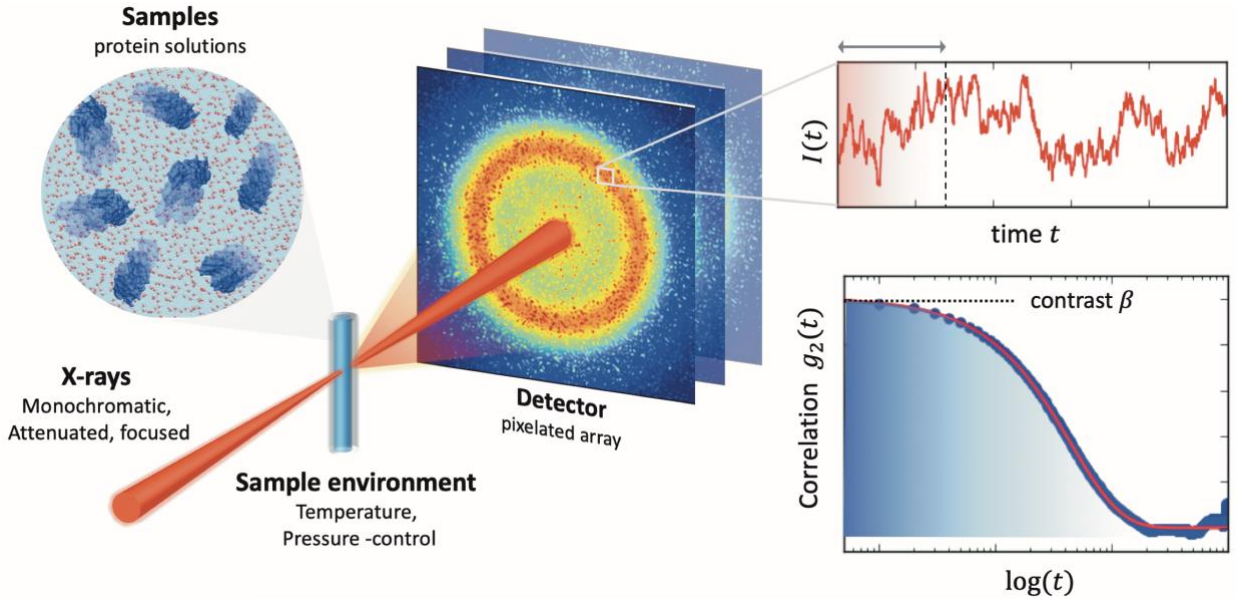

Figure 1. A typical experimental setup of X-ray Photon Correlation Spectroscopy (XPCS). The scattering intensity is recorded with a pixelated 2D array detector. The scattering intensity is recorded as a function of time, which fluctuates due the changes of the speckle pattern (upper right-hand panel). 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 b and the decay constant reflects the timescale of motion associated with the given momentum transfer Q.

[1] F. Perakis, K. Amann-Winkel, F. Lehmkühler, M. Sprung, D. Mariedahl, J. A. Sellberg, H. Pathak, A. Späh, F. Cavalca, D. Schlesinger, A. Ricci, A. Jain, B. Massani, F. Aubree, C. J. Benmore, T. Loerting, G. Grübel, L. G. M. Pettersson and A. Nilsson, Proc. Natl. Acad. Sci. U.S.A. 114, 8193-8198 (2017)

[2] F. Perakis, G. Camisasca, T. J. Lane, A. Späh, K. T.Wikfeldt, J. A. Sellberg, F. Lehmkühler, H. Pathak, K. H. Kim, K. Amann-Winkel, S. Schreck, S. Song, T. Sato, M. Sikorski, A. Eilert, T. McQueen, H. Ogasawara, D. Nordlund, W. Roseker, J. Koralek, S. Nelson, P. Hart, R. Alonso-Mori, Y. Feng, D. Zhu, A. Robert, G. Grübel, L. G. M. Pettersson, and A. Nilsson, Nature Comm. 9, 1917 (2018)

[3] F. Perakis and C. Gutt, Phys. Chem. Chem. Phys., 22, 19443-19453 (2020)

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