



**Thursday, 18 November 2021, 10:00 – 11:00**

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**Structure and damage of disordered materials:  
opportunities for XFEL science**

The structural characterization of disordered matter poses fundamental challenges. Crystallography solves the “structure problem” for crystals by producing detailed 3D images and, from those structures, properties can be predicted accurately. No such method exists for disordered materials. For a start, disordered structures don’t have a single atomic structure, but an ensemble. Secondly, X-ray or electron diffraction methods yield structural models that make differing predictions about material properties. XFELs provide small, powerful beams to measure 3D information from disordered matter. This includes liquids, where XFELs could outrun molecular diffusion. Fluctuation scattering techniques provide an advanced statistical approach to extract this 3D information. We have developed the pair-angle distribution function (PADF) technique to map this information in real-space. We will discuss the prospects of the PADF at XFELs to study liquids and protein crystallization in 3D. XFELs also generate disorder in all samples via complex ionization cascades. Modelling this damage is key in any new demonstration of a new structural technique, but also computationally expensive. We will present work on a new approach to modelling XFEL damage using a hybrid of molecular dynamics and plasma-based models, with an aim to speeding up calculations for larger systems.

**Host: Nils Brouwer**

Zoom link:

<https://xfel.zoom.us/j/99279524796?pwd=V2toRnU5SkkwNWJGL0xDmFKTGMwUT09>  
Meeting ID: 992 7952 4796  
Passcode: 378634