CHYN MEETS HARBOR

Overcoming the limitations of high-resolution structural biology

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and

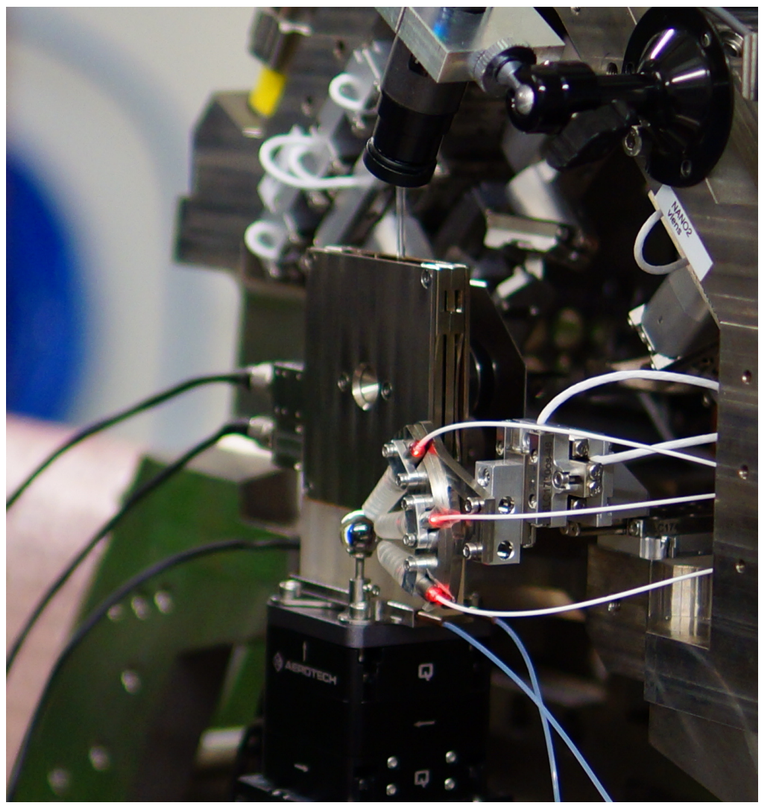
Live View of Nanomaterials Chemistry

Lukas GROTE

Abstract Talk 1: For over 50 years, X-ray crystallography has been the primary method to determine the structures of biological macromolecules. Even with over 100 000 known structures, it still has limitations: Some biological questions - for example whether a certain ligand is bound - cannot be answered, as the electron density map gives no clear indication; some structures, such as membrane proteins and large complexes cannot be solved; and worst of all, published and seemingly correct structure solutions can have integral flaws that might even bring about complete retraction of a structure and the associated publications. There is a fundamental problem underlining all of these problems: the large discrepancy between the measured X-ray diffraction data and the molecular models we employ to interpret these data. This discrepancy is typically measured as a percentage called the R (or residual) value. While small molecule structures routinely reach R-values of 5%, macromolecular structures typically are about 25%. What causes this gap? In this talk, I will describe our search for an answer to this question, which led to the development of new data quality diagnostics for XFEL and other diffraction data (www.auspex.de), a neuronal network for Cryo-EM maps and finally to the realization that something might be fundamentally missing from the atomic models we employ to interpret diffraction data.

Abstract Talk 2: Nanomaterials with well-controllable structure are of particular interest in many fields of research, and knowledge on their formation mechanism and structural evolution is essential for developing precise chemical synthesis routes. To this end, X-ray ptychography, a scanning coherent diffraction imaging (CXDI) technique, can be used to record micrographs inside a chemical reactor, following a solution based synthesis in real time. With state-of-the-art nano focused beams, a spatial resolution of 20 nm can be achieved even when imaging weakly scattering objects.

I will briefly introduce the Ptychographic Nanoanalytical Microscope (PtyNAMi) at the nanofocus endstation of beamline P06 at PETRA III, and present a sample environment for running chemical syntheses in the X-ray beam. The dynamics of Kirkendall void formation in Cu_2O nanocubes during chemical reduction to metallic copper, and the formation of hollow gold nanostructures by galvanic replacement of Cu_2O nanocubes are two examples that can benefit from the proposed nanoimaging approach.



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