crystals [1,2]. The focus of structural biology is turning towards challenging protein complexes that most frequently give very small crystals. This will obviously increase the demands for pushing the limits of the diffraction experiments, .and create a foreseeable need for macromolecular crystallography beamlines with X-ray beams a few μm in size and even smaller. Positioning of μm sized samples in an X-ray beam of the same dimension necessitates use of beamline instrumentation with an order of magnitude higher precision that is available presently. Meeting these challenges in instrumentation requires an integrated approach to the development of micro- and nanofocussing optics, sample handling and positioning. In addition to pushing the diffraction experiment to the limits, examples will be given on how the micro- to nanometer sized synchrotron beams can be employed with other complementary experimental techniques, that contributes to the overall insight in structural-functional relationships of biological systems.

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Keywords: synchrotron radiation, protein structures, microbeam

KN05

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Photochromism of diarylethene single crystals-reversible color and shape changes on photoirradiation

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Photochromism is defined as a reversible transformation between two forms having different absorption spectra on photoirradiation. Although a large number of photochromic compounds have been so far reported, compounds which exhibit photochromism in the crystalline phase are rare. During the course of study on photochromism of diarylethenes we found some derivatives undergo thermally irreversible photochromic reactions even in the single crystalline phase (1). Very high photocyclization quantum yields, close to 1, and very low activation energy, close to zero, were found in the crystalline photochromism (2). A single crystal containing three different kinds of diarylethene derivatives was prepared. The crystal exhibited various colors, yellow, red and blue upon irradiation with light of appropriate wavelengths (3). Colored forms were stable in the crystal even at 100℃ and the coloration/decoloration cycles could be repeated more than 10,000 times. The photochromic diarylethene crystals showed not only the color changes but also reversible surface morphology and shape changes on alternate irradiation with UV and visible light (4). Small geometrical structural changes of the molecules induced by light in the crystal caused the morphology and shape changes. The single crystals based on diarylethenes and with size ranging from 10 to 100 micrometers exhibited rapid and reversible macroscopic changes in shape and size induced by UV and visible light (5).

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Keywords: photochromism, diarylethene, photomechanical effect

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Quantum simulations of liquids and solids under pressure: Synergy between theory and experiment

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We will discuss progress and challenges in the investigation of systems under pressure, using quantum simulations. In particular, we will focus on low-Z solids and liquids and present recent results on the phase diagram of hydrogen, carbon and water.

Keywords: low-Z solids and liquids, quantum simulations, carbon, hydrogen, water

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Cryoelectron tomography: From molecules to systems

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Electron Tomography (ET) is uniquely suited to obtain 3-D images of large pleiomorphic structures. While the principles of ET have been known for decades, its use has gathered momentum only in recent years. Technological advances have made it possible to develop automated data acquisition procedures. This, in turn, allowed to reduce the total electron dose to levels low enough for studying radiation sensitive biological materials embedded in vitreous ice. As a result, we are now poised to combine the power of high-resolution 3-D imaging with the best possible preservation of the specimen. ET of frozen-hydrated prokaryotic cells or thin eukaryotic cells provides 3-D images of macromolecular structures unperturbed and in their functional environment at molecular resolution (2-4 nm). Such tomograms contain vast amounts of information; essentially they are 3-D images of the cell's proteome and they should ultimately enable us to map the spatial relationships of macromolecules in a cellular context. However, it is no trivial task to retrieve this information because of the poor signal-to-noise ratio of such tomograms and the crowded nature of the cytoplasm. Advanced pattern recognition methods are needed for detecting and identifying specific macromolecules based on their structural signature. Provided that high- or medium-resolution structures of the molecules of interest are available, they can be used as templates for a systematic interrogation of the tomograms. Once the challenges of obtaining sufficiently good resolution and comprehensive libraries of template structures become available, we will be able to map the supramolecular landscape of cells systematically.

Keywords: electron tomography, visual proteomics, macromolecular complexes

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Advances in direct-space structure determination of molecular materials from powder diffraction data

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