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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2. Michael R. Sawaya et al Nature 447 (2007) 453-457.

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

KN06

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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

KN07

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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

KN08

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

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Many crystalline solids can be prepared only as microcrystalline powders and are not suitable for structural characterization by single-crystal X-ray diffraction methods. For such materials, it is necessary instead to tackle structure determination using powder X-ray diffraction data. Although there have been several successful reports of the structure determination of organic molecular solids using traditional strategies for structure solution from powder X-ray diffraction data, the majority of recent work on such materials has exploited the direct-space strategy for structure solution, followed by Rietveld refinement. Indeed, the recent upsurge of activity in this field (in both academic and industrial sectors) has taken place closely in parallel with the development of the direct-space strategy for structure solution, for which a range of different computational implementations are now available. In the direct-space strategy, a hypersurface defined by an appropriate R-factor (in our case the powder profile R-factor) is searched using an appropriate global optimization technique (such as Monte Carlo, simulated annealing or Genetic Algorithm techniques). Our recent research is focused on the development, optimization and implementation of Genetic Algorithm techniques in this field, as well as the application of these techniques to solve the crystal structures of a wide range of different types of molecular materials from different areas of the solid state and materials sciences. The lecture will describe fundamental aspects of the direct-space strategy for structure solution from powder X-ray diffraction data, and will be illustrated by examples selected to highlight the current scope and potential for the application of techniques in this field.

Keywords: structure solution, powder diffraction, molecular solids

KN09

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Powder diffraction studies of proteins

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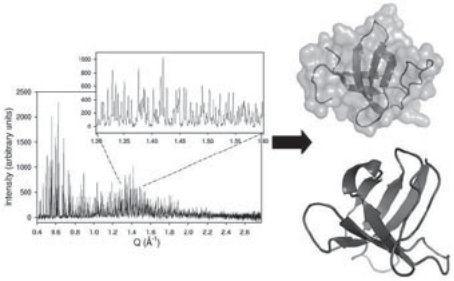
Studying biological macromolecules in the absence of good quality single crystals is a challenging field attracting considerable scientific interest. Modern developments of X-ray powder diffraction have allowed the structural investigation of a range of proteins establishing the method as a useful complementary tool to traditional approaches [1]. Protein powder specimens consist of a large number of randomly oriented diffracting micro-crystals which are usually formed rapidly by batch crystallization under a variety of conditions. An overview of the most recent developments in this field will be presented including: (a) application of the molecular replacement technique and structure refinements of selected proteins (b) methods for successful cryocooling (c) experimental phasing and extraction of molecular envelopes (d) high throughput automated data collection allowing systematic investigations such as screening and phase diagram mapping and (e) application of the method on biologically interesting proteins. Practical applications of the methods will be illustrated by recent examples.



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Keywords: protein crystallography structures, powder crystallography, synchrotron structural biology research

KN10

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Structural biology studies of the avian influenza H5N1 virus

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Highly pathogenic avian influenza A virus strains with H5N1 subtype are entrenched in poultry worldwide and pose a growing threat to human health. Of the 382 reported human cases of avian influenza since 2003, 241 have been fatal. The development of novel anti-influenza therapeutics is vital in order to increase preparedness against a global influenza pandemic. To this end, we initiated a structural biology program in China to systematically study the proteins from the avian H5N1 influenza A virus (A/goose/Guangdong/1/96). Our aims are to understand the underlying mechanisms of viral replication and the interaction of the virus with host cell factors. Here I will report some exciting recent progress in our efforts.

Keywords: avian influenze H5N1, crystal structure, drug target

KN11

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The crystallochemical basis of synthetic mineral immobilisation technologies

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The selection of synthetic mineral immobilisation matrices for the treatment of inorganic pollutants is governed by several considerations. First, toxic metals should be incorporated in their least harmful chemical states. For example, As^{3+} and Cr^{6+} are less poisonous than As^{5+} and Cr^{3+}. Second, as it may be necessary to simultaneously accommodate the oxidized and reduced species of different metals, the suite of mutually compatible minerals that can be selected is restricted. Third, structures with multiple cation and/or anion acceptor sites minimize the number of phases required to crystallise simultaneously, and allows greater flexibility to respond to variations in waste stream composition. This, in turn, limits the chance of undesirable compounds forming. Finally, phases with the highest proportions of appropriate cation acceptor sites are advantageous, to achieve high waste loadings with less 'bulking' through the introduction of inert additives. Within these constraints, a subset of structural families - perovskite, spinel, apatite, zirconolite, zeolites, clays - form the basis of many synthetic mineral immobilisation technologies. The crystallochemical properties of these waste forms are complex and remain the subject wide investigation. The final products are usually far from thermodynamic