KN01

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What Protein Data Bank tells us about the past, present, and future of structural biology

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When the Protein Data Bank (PDB) archive was established in 1971 with seven structures, it was difficult to predict what the future of structural biology was going to look like. Now with more than 50,000 structures in the archive, it is possible to discern patterns that provide an informative view of the progress of structural biology through the years. The current PDB reflects many positive outcomes. Many structures are larger and more complex. Structures that were once thought impossible to determine (such as ribosomes, large viruses, and enzyme complexes) are now commonplace. Using the power of high throughput crystallography, the structural genomics projects have produced a large number of new and novel structures, with many presenting us with the challenge of functional annotation. New and hybrid methods are being used in structure determinations. No longer limited to structural biologists, the PDB user community has grown to include scientists working on basic and applied research in various fields, students, educators, and general audiences. By analyzing the contents of the PDB archive, it is also possible to decipher trends that allow us to prepare for a future in which biology and medicine can be described increasingly in molecular terms. The PDB archive is managed by the Worldwide Protein Data Bank (wwpdb.org).

Keywords: protein structural relationships, structural databases, protein structure database

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Ab-initio powder diffraction studies of organometallics and coordination polymers

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Crystal structure solution from powders data may play a central role in research and technology allowing the characterization of materials which are not available as single crystals of adequate size and quality. Owing to the collapse of the three-dimensional lattice onto the 2 θ axis, ab-initio crystal structure solution was considered quite a challenge. However, the usage of brute force Montecarlo approach (for searching parameters space) and of Single Value Decomposition (for solving linear equations relating hkl values to d-spacings) has greatly increased the probabilities of indexing large unit cells even in the presence of impurities.[1] Similarly, global optimization methods have greatly enhanced the scope of powder diffraction whenever the sampling of the most proper 'chemical' space is granted by suitable structural hypotheses. [2]Direct-space strategies allow the determination of moderately large crystal structures (even from non-indexed low-quality X-ray powder patterns)[3] but are intrinsically biased by the large amount of previous 'knowledge' required. The role of complementary information[4] in the formulation of the starting structural model and its validation[5] will be discussed in the light of our work on organometallics [4] and metal diazolates. [6]

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Keywords: *ab-initio* powder structure determination, organometallic polymers, framework structures

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Growth of silica biomorphs: Self-assembled crystal aggregates with non-crystallographic morphologies

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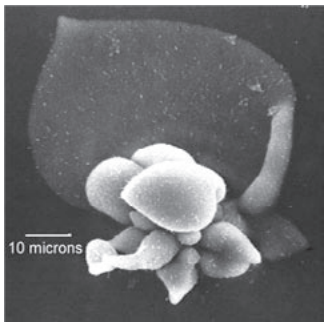
Bizarre as it might seem, purely inorganic processes may yield self-assembled crystal aggregates displaying morphologies that, like those produced by living organisms, are not controlled by crystallographic symmetry. An amazing example is the formation of silica biomorphs, a synthetic material that share with life complexity, morphology, hierarchy and self-organization yet it is remarkably simple in chemical terms (see Figure). The synthesis requires only a source of carbonate ions (e.g. atmospheric CO_2) strong alkaline aqueous solutions, silica and alkaline-earth cations (Ba and Sr, Ca) at room temperature. Under these conditions, the precipitation of alkaline-earth carbonates coupled with silica interactions yields crystal aggregates made of millions of nanocrystals exhibiting self-assembled non-crystallographic morphologies (J.M. Garcia-Ruiz. Geology 26 (1998) 843; J.M. Garcia-Ruiz, et al., Science 302 (2003) 1194). I will review in this paper the present knowledge on the morphological and textural properties of silica biomorphs and the morphogenetical process accounting for the formation of these complex self-organized crystal aggregates.



Keywords: crystalline morphology, biomimetics, biomaterials development

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The role of micrometer sized synchrotron radiation beams in the development of structural biology

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Micrometer sized synchrotron radiation beams have opened new possibilities for structure determination of molecules that previously were inaccessible as they formed very small and weakly diffracting

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

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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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