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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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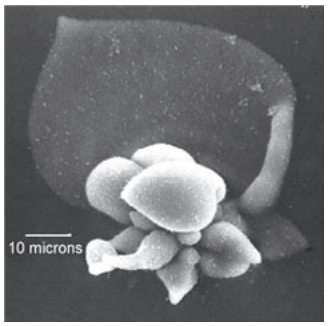
Bizarre as it might seem, purely inorganic processes may yield self-assembled crystal aggregates displaying morphologies that, like those produced by living organisms, are not controlled by crystallographic symmetry. An amazing example is the formation of silica biomorphs, a synthetic material that share 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