

buffer (PB) (pH 7.0) containing 0.1 M NaCl. Solution SAXS measurements were carried out at the BL45XU RIKEN Structural Biology Beamline I (wavelength, $\lambda = 0.09$ nm) of the SPring-8, Harima, Japan. Two-dimensional (2D) SAXS images were recorded with a CCD camera. For aggregation experiments, the complementary DNA and then NaCl were added to the suspension in such a way that the final concentrations of complementary DNA and NaCl were 0.5 μ M and 1 M, respectively.

The non-crosslinked assembly has a crystalline structural order but less long-range ordering. The inter-surface distance between the particles increased with the length of dsDNA. From the experiments using the binary mixtures, it was unveiled that the DNA-functionalized particles with the same core size assemble together irrespective of tethered DNA. Furthermore, it was demonstrated that, for smaller core sizes or longer DNA lengths, their nanoparticles covered with full-matched dsDNA can disperse stably above a temperature which is lower than the melting temperature of the dsDNA. This may cause by steric stabilization of DNA molecules. It is considered that the attractive interaction in the non-crosslinking aggregation is attributable to van der Waals potential between core particles, and the contribution of the end-to-end stacking attraction between dsDNA might be little. As a plausible mechanism, the feature of non-crosslinking aggregation interaction could be characterized by steric repulsion stabilization due to entropic loss in conformation and mobility of DNA molecules.

Keywords: DNA, colloid, SAXS

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Further development of Brillouin zone database on the Bilbao Crystallographic Server

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The Bilbao Crystallographic Server (www.cryst.ehu.es) [1] is a web site offering online crystallographic programs and databases. The aim of this contribution is to announce the modifications and improvements of the Brillouin zone database available on the server. The database includes Brillouin zone figures (fig. 1) and tables of the wave-vectors for all space groups that form the background of the classification of the irreducible representations of all 230 space groups. The wave-vectors of reciprocal space are classified in terms of their symmetry described by the symmorphic space groups available in Volume A of *International Tables for Crystallography* (ITA). This is possible due to the isomorphism between the reciprocal space groups, describing the symmetry of the wave-vectors, and the symmorphic space groups in direct space [2]. In the database, the ITA-classification scheme is compared with the classification of the wave-vectors available in the tables of space-group representations by Cracknell, Davies, Miller and Love [3].

The recent modifications of the database have been focused on a general improvement and homogenization of the stored data and a clearer presentation of the Brillouin-zone figures. The wave-vector tables list for each space group the coordinates of the wave-vectors with respect to primitive (CDML) and conventional dual bases compared with the coordinates according to the ITA description. The Brillouin-zone figures for trigonal, hexagonal and rhombohedral space groups are redrawn applying a much more visual clinographic projection, which was also used for the rest of the space groups. The figures and tables for monoclinic space groups in *unique axis b* setting have been also included in the database.

In addition, we have developed a computer tool for the complete

characterization of the wave-vectors: given the wave-vector coordinates referred to primitive or conventional dual bases, the program assigns the corresponding wave-vector symmetry type, specifies its CDML label, determines the little co-group of the wave-vector and generates the arms of the wave-vector star.

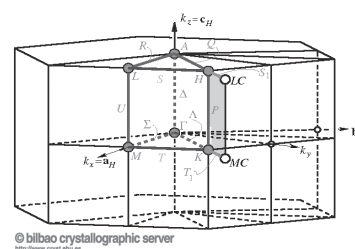


Figure 1: Brillouin-zone diagram for the space groups of the arithmetic crystal class 6/mmmP

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The wwPDB common tool for deposition and annotation

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An early example of open data sharing, the PDB archive has provided the research community with information about the 3D structures of biological macromolecules for the past 40 years. From 7 structures in 1971 to more than 70,000 in 2010, PDB data are used by researchers in academia, government and industry, and educators.

The Worldwide Protein Data Bank (wwPDB; wwpdb.org) consists of four organizations from the USA, Europe, and Japan that together curate and disseminate the single, global PDB archive of biomacromolecular structures. The wwPDB is committed to using the highest standards of curation and validation to process experimental 3D biomolecular structure data.

The next 10 years will bring several challenges for this repository including significant increases in throughput and in the size and complexity of structures being deposited. In response to this challenge the wwPDB has initiated the *Common Deposition and Annotation Tool* project to produce the next generation of processes and tools. This new system will be used at all wwPDB sites to curate structural data produced by any combination of experimental techniques (X-ray, NMR, EM) to support the wwPDB goals of quality and dependability over the next 10 years. The new tools are designed to fulfill the goals of high standards of curation quality and dependability and to add value to depositors as they interactively deposit new structures. The