

Poster Sessions

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Keywords: tubulin, chaperons, electron microscopy.

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Structures of a group II chaperonin.

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Thermosomes are group II chaperonins responsible for protein refolding in an ATP-dependent manner. Little was known regarding the conformational changes of thermosomes during their functional cycle due to lack of high-resolution structure of open state. We reported the first complete crystal structure of thermosome (rATcpn β) in open state from *Acidianus tengchongensis*. There is a $\sim 30^\circ$ rotation of the apical and lid domains compared to the previous closed structure. Besides, the structure reveals a conspicuous hydrophobic patch in the lid domain and residues locating in this patch are conserved across species. Both the closed and open forms of rATcpn β were also reconstructed by electron microscopy (EM). Structural fitting revealed the detailed conformational changes from open to closed state. Structural comparison as well as protease K digestion indicated only ATP binding without hydrolysis does not induce chamber closure of thermosome.

Besides, we have solved a lot of cryoEM structures of rATcpn in different assemblies and functional states with different conformations using data collected on Titan Krios. We discovered that the cooperativity between heterologous subunits is indispensable for the performance of complete chaperonin function and clarify the structural basis for the functional cooperativity.

Keywords: thermosome, crystallography, cryoEM

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The structure of the *in vivo* assembled CCT:G protein $\beta 1$ subunit complex reveals a novel CCT substrate binding mechanism mediated by hydrophobic interactions

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The eukaryotic cytosolic chaperonin CCT/TriC plays a crucial role in the folding of a set of very important proteins [1]. The CCT substrate recognition mechanism has been found, in the case of the cytoskeletal proteins actin and tubulin, to be based on specific interactions involving

charged and polar residues of both the chaperonin and the unfolded substrate. Here we show for the first time the three-dimensional reconstruction of the complex formed by CCT and the G protein β_1 subunit, isolated *in vivo* from insect cells. G β_1 represents the major class of CCT substrates, the WD40 repeat proteins that form β -propeller structures [2]. The electron microscopy analysis reveals that G β_1 interacts specifically with the apical domain of CCT β . G β_1 binding experiments with several CCT chimeric proteins confirm the specific interaction with CCT β and map G β_1 binding to a hydrophobic core of amino acids located in α -helix 9 and in the loop between β -strands 6 and 7, facing the chaperonin cavity. From these results, a model for the folding of G β_1 mediated by CCT and its co-chaperone PhLP1 is proposed.

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Self-assembly of copolymers containing a polypeptide block

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The self-assembly of PEGylated peptides containing a modified sequence from the amyloid β peptide, FFKLVFF, has been studied in aqueous solution [1]. PEG molar masses, PEG1k, PEG2k and PEG10k were used in the conjugates. It is shown that the three FFKLVFF-PEG hybrids form fibrils comprising a FFKLVFF core and a PEG corona. The β -sheet secondary structure of the peptide is retained in the FFKLVFF fibril core. At sufficiently high concentrations FFKLVFF-PEG1k and FFKLVFF-PEG2k form a nematic phase, while PEG10k-FFKLVFF exhibits a hexagonal columnar phase. Simultaneous small angle neutron scattering/shear flow experiments were performed to study the shear flow alignment of the nematic and hexagonal liquid crystal phases. On drying, PEG crystallization occurs without disruption of the FFKLVFF β sheet structure leading to characteristic peaks in the x-ray diffraction pattern and FTIR spectra. The stability of β -sheet structures was also studied in blends of FFKLVFF-PEG conjugates with poly(acrylic acid) (PAA). While PEG crystallization is only observed up to 25 % PAA content in the blends, the FFKLVFF β -sheet structure is retained up to 75% PAA in FFKLVFF-PEG/PAA blends.

[1] V. Castelletto, G.E. Newby, I.W. Hamley, L. Noirez, *Langmuir* **2010**, *26*, 9986-9996.

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Ionic liquids (IL): structures model

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There are two opposite opinions on the structure of IL: on one

hand, structural heterogeneities (domains) are real (either alkyl groups or groups of ions), on the other hand, structural heterogeneities result from erroneous interpretations of experimental data. Structural heterogeneities are considered to determine all properties of IL as dissolution, solvation rate, self-diffusion, diffusion of substances dissolved in IL, electron transport etc. IL structures were investigated by SAXS and WAXS methods, by diffraction of synchrotron radiation and neutrons followed by interpretation of the radial distribution functions by molecular dynamic simulations. Structural model of IL is not available now in spite of the active research and great demand for such model. IL structure model shortly presented below is based on literature experimental data for imidazolium and tetraalkylammonium ILs with cation:anion ratio 1:1.

In accordance with the suggested model, 4 cations and 4 anions form an octupole and alkyl tails belonging to the neighbour octupoles are combined in pairs giving hydrocarbon domains. Octupoles and alkyl domains are two structural heterogeneities which construct IL structure. Octupoles are distributed in place of carbon atoms in the diamond structure and two diamond structures are inserted in one another with a shift for a half of the cubic cell dimension (diamond structure is friable so octupoles of one diamond structure fill the voids of another diamond structure). Alkyls are arranged along the C-C bond in diamond structure. Diamond-like cubic structure of IL can't help containing fragments of lonsdaleite structure and intermediate configurations. That is one of important reasons for the long range order absence.

Octupole combination of cations and anions is confirmed for alkylammonium (alkylphosphonium) IL. Nitrogen (phosphorous) atoms of four cations are distributed upon cube vertexes and three alkyl chains of each cation are situated above the face diagonal of the cube, i.e. pairs of alkyls are formed above one of two diagonals of any cubic face what means the alkyl domain existence. Four more vertexes of the cube are occupied with anions forming an octupole together with four cations. The fourth alkyl chain of each cation is oriented off the cube along the three-fold axis of octupole. The nearest octupoles combine such alkyls in pairs in the diamond-like (lonsdaleite-like) structures similarly to imidazolium IL. The suggested model is close to the structure of concentrated solutions of electrolytes.

Keywords: ionic, liquid, model

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The crystal engineering approach to design the pheromone releasing LMWG

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Gels are ubiquitous in nature and in everyday life. Starting from protoplasm to shaving cream, all are gel. It is a visco-elastic soft material comprising of a small amount of solid and a huge number of organic (organo gel) or aqueous (hydro gel) solvent(s). In a typical experiment, a relatively dilute solution of a gelator is heated and cooled below the critical temperature (sol-gel transition temperature), the immobilization of solvent occur by withstanding its own weight is termed as gel [1]. Under several kind of microscopic observation, it is found that, 1D self assembled fibrillar network (SAFIN) are cross linked among themselves via junction zones to form 3D matrix to arrest the flow of solvent. As SAFINs are the key to gel formation,

it is very important to investigate its molecular level self assembling by analyzing the crystal structure. It is not possible to obtain an x-ray crystal structure in its native state, as submicrometer size SAFINs are very poorly diffracting along with the scattering contribution of solvent molecules. Ab initio crystal structure determination of SAFIN using x-ray powder diffraction (XRPD) with very slow scan speed may be an alternative one but such a method of structure determination is not routine yet and requires high-intensity synchrotron beams, which are not readily accessible.

However, it was proposed by Shinkai nearly a decade ago that 1D hydrogen bonded networks promotes gelation whereas 2D and 3D networks either produce weak gels or no gelation at all. The fact that this hypothesis was indeed based on a logical foundation was most explicitly demonstrated by us by exploiting supramolecular synthons, which was first proposed by Desiraju in *Crystal Engineering*. We have identified and exploited some supramolecular synthones, namely Primary Ammonium Monocarboxylate (PAM), Primary ammonium Dicarboxylate (PAD), Secondary Ammonium Monocarboxylate (SAM) and Secondary Ammonium Dicarboxylate (SAD) synthons, which are robust enough to produce 1D hydrogen bonded network (HBN) with desired fictionalization.

Easy access to a class of chiral gelators has been achieved by exploiting primary ammonium monocarboxylate (PAM), a supramolecular synthon. A combinatorial library comprising of 16 salts, derived from 5 lamino acid methyl esters and 4 cinnamic acid derivatives, has been prepared and scanned for gelation. Remarkably, 14 out of 16 salts prepared (87.5% of the salts) show moderate to good gelation abilities with various solvents. Anti-solvent induced instant gelation at room temperature has been achieved in all the gelator salts, indicating that the gelation process is indeed an aborted crystallization phenomenon. Rheology, optical and scanning electron microscopy, small angle neutron scattering, and X-ray powder diffraction have been used to characterize the gels. A structure-property correlation has been attempted, based on these data, in addition to the single-crystal structures of 5 gelator salts. Analysis of the FT-IR and ¹H NMR spectroscopy data reveals that some of these salts can be used as supramolecular containers for the slow release of certain pest sex pheromones. The present study clearly demonstrates the merit of crystal engineering and the supramolecular synthon approach in designing new materials with multiple properties.

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Keywords: crystal engineering, supramolecular synthon, sex pheromones

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Structure of a new μ -oxalic acid- μ -oxalato -dicaesium, Cs₂(H₂C₂O₄)(C₂O₄) at 100K

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As a part of our study concerning the polymeric metallic dicarboxylates, their supramolecular features and their fascinating and attractive architectures, several oxalato-based alkali metal have been obtained as monometallic as well as bimetallic single crystals with Rb [1], [2], Li and Cs atoms. For the two first alkali metals, the structural investigations have conclude that the corresponding compounds have the specificities of coordination polymers .

Concerning the Cs atom, two oxalato-based compounds have been previously reported, one formed with the partially deprotonated acid CsHC₂O₄ [3] and the other containing both partially deprotonated