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Keywords: membrane proteins, electron crystallography, methods development

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Atomic Model of Microsomal Glutathione Transferase 1 from Electron Crystallography
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The integral membrane protein microsomal glutathione transferase 1 (MGST1) possesses glutathione and peroxidase activity thus protecting the organism from toxic substances. We have determined the atomic model of MGST1 at 3.5Å resolution by electron crystallography of 2-dimensional crystals from two different two-sided plane groups making it the first membrane enzyme solved to atomic resolution by this technique. The MGST1 homotrimer is constructed by 12 trans-membrane helices forming three all alpha-up-down 4-helix bundles with a fold strikingly similar to the cytochrome c oxidase subunit I suggesting divergent evolution from a common structural ancestor. The MGST1 model reveals inter-subunit interaction and strengthens previous suggestions of global conformational changes upon glutathione (GSH) binding. Furthermore a possible location of the putative hydrophobic binding site is suggested.
Keywords: microsomal glutathione transferase 1, membrane protein structure, electron crystallography

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Structural Features of Cyclodextrin Inclusion Complexes
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Inclusion complexes of α-,β- and γ-cyclodextrins with poly(ethylene glycol)(PEG) and other polymers were prepared using various methods reported so far. The inclusion complexes exhibited the following crystalline features.

1.The inclusion complex of α-cyclodextrin/poly(ethylene gycol) gave a very spotty hexagonal electron diffraction pattern, which gave the hexagonal unit cell. In the case ofβ-cyclodextrin/ poly(propylene glycol), a spotty hexagonal electron diffraction pattern was also observed. The spotty appearance of these electron diffraction pattern is caused by the following host/guest arrangement: The host cyclodextrin columns are arranged in ordered way, even though guest molecules randomly oriented in the caves of dextrin hosts.

2.The inclusion complexe of γ-cyclodextrin with poly(ethylene adipate) gave a "superlattice" comprising 8x8 cyclodextrin units, and additionally its electron diffraction pattern showed the characteristic streaky diffuse scattering due to the attacking fault of the cyclodextrin units.

3.The inclusion complexes contained water molecules in them. The crystal structure was largely disordered, when water molecules were removed by heat treatment. As the original structure was recovered by exposing water vapor, the structural order/disorder transition occurs reversibly.
Keywords: cyclodextrin, superlattice, electron diffraction

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In-situ X-ray Scattering Studies of Nanomaterial Growth Dynamics in Aerosols
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Nanomaterials display unique properties intermediate between those of the molecular and macroscopic regimes. The interest in application of nanomaterials has driven a desire to understand the fundamental mechanisms and processes involved in nanomaterial formation. Generally, nanomaterials are formed under non-equilibrium conditions with deep supersaturation and are commonly formed by extremely rapid growth processes that lead to kinetically dominated structural features. Aerosols offer transient and dramatic changes in temperature, concentration and stoichiometry that can be put to use to produce highly non-equilibrium conditions for nanomaterial formation. Our understanding of nanomaterial formation under these conditions can be studied in situ using synchrotron based techniques. This presentation will highlight some of the most important discoveries made during the past 2 years at ESRF and APS (USA) on flames and environmental aerosols. The work was supported by the Swiss National Science Foundation, the US National Science Foundation and Dupont Corporation.

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Dynamics of Amphiphilic Systems Probed by Highly Time-resolved SAS Experiments
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Amphiphilic molecules form a large variety of self-aggregating structures that are highly dynamic with time scales ranging from μs to weeks. Often morphological changes can be triggered by mixing with other surfactants, additives, or solubilisates. In our experiments rapid mixing was studied by coupling the stopped-flow technique to high-flux SANS/SAXS instruments which allows to obtain detailed structural information with a time-resolution of 5-50 ms. By this method a large variety of different structural transitions were investigated, e. g. the formation of unilamellar vesicles by admixing oppositely charged surfactant or a cosurfactant. For both cases slow formation of monodisperse unilamellar vesicles is observed that takes place in a way purely governed by diffusion. Both, kinetics and the final structure depend strongly on the electrostatic conditions of the system. In other experiments the disintegration of micelles when mixing with a bad solvent was followed, which passes through a minimum aggregation stage before smaller micellar structures are reformed. This applies also to much larger block copolymer micelles of the PIB-PAA type. Their response to changes of ionic strength and also their complexation with oppositely charged polyelectrolytes was studied. For all cases the details of the transformation can be studied and in particular it is possible to identify intermediate structures, a point which is very important for a systematic control of the dynamics of self-aggregating systems.
Keywords: colloids, amphiphilic molecules, dynamics

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Cytochrome C and αTS Folding Probed by Submillisecond Continuous-Flow SAXS
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