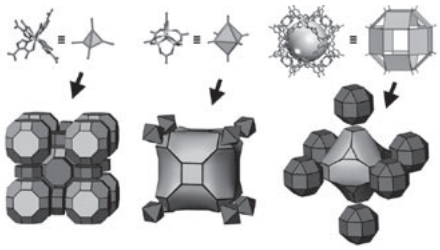
highly functional character. The molecular building block (MBB) approach introduces the ability to generate rigid and directional building blocks, mostly *in situ*, for the construction of MOMs having specific underlying networks and/or targeted functions/properties. Here we will discuss three basic strategies based on the MBB approach. Three classes of MBBs can be targeted and utilized in the assembly of functional MOMs: 1) single-metal-ion-based MBBs, which promote the rational construction, by forcing rigidity and directionality through control of the metal coordination sphere and judicious selection of suitable hetero-functional (N-, O- coordination) organic ligands, of porous MOMs with extra-large cavities, including zeolite-*like* metal-organic frameworks (ZMOFs); 2) multi-nuclear metal cluster-based MBBs, where, for example, simple metal-carboxylate clusters possess multiple metal-oxygen coordination bonds that result in the generation of rigid nodes with fixed geometry that, when combined with organic ligands of specific geometry, lead to the construction of desired MOMs (e.g. *soc*-MOFs); and 3) supermolecular building blocks (SBBs), which involve enhanced built-in directional and structural information (e.g. high degree of symmetry and connectivity) compared to simple MBBs and allow the construction of high-connectivity nets (e.g. *rht*-MOFs). The MBB approach and associated strategies, as well as physical properties of some corresponding MOMs, will be presented.



KN30

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Atoms and spins in novel multiferroics: A new twist to an old relation

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In the broadest interpretation, multiferroics are materials that display complex ordering phenomena, with at least two coupled order parameters capable of responding to different external fields. Magneto-electric multiferroics in particular have an obvious appeal as functional paradigms, since they display coupled responses to electrical and magnetic fields, and can therefore be "switched" and "read" with different external stimuli and probes. Recently, an entirely family of "novel" multiferroics has emerged, in which, unlike conventional multiferroics, the onset of electrical polarization coincides with a magnetic ordering transition. Many of these materials have been known for decades, often as "odd" examples of complex antiferromagnets, but they multiferroics properties were completely overlooked. The attractive feature of these systems is not so much the electrical polarization, which is several orders of magnitude smaller than for typical ferroelectric but rather the very large cross-coupling between magnetic and electrical properties. The key to understand these remarkable effects lies on one hand in the magneto-elastic interactions coupling spins, atoms and electrons at the microscopic level, and, on the other hand, in the subtle lowering of the magneto-crystalline symmetry from a non-polar to a polar point group. Crystallography, intended as the study of symmetry and of the normal modes that break it systematically, continues to play a starring role in the study of novel multiferroics. I will present a number of examples to show how the crystallographic determination of the atomic and spin structures and their evolution with temperature, pressure, magnetic and electric field has provided compelling evidence to unravel the physics of multiferroics.

Keywords: multiferroics, magnetic structures, phase transitions

KN31

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Structure of the FhaC translocation pore : Insights into transport across the bacterial membrane

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The superfamily of Omp85/TpsB membrane proteins includes essential proteins such as the Toc75, Sam50/Tob55 and Omp85/YaeT homologs, which are the cores of large hetero-oligomeric complexes involved in protein transport across, and insertion of beta-barrel proteins into, the outer membrane of chloroplasts, mitochondria and Gram-negative bacteria. It also includes TpsB transporters, which are components of the "Two-Partner Secretion" (TPS) systems in Gram negative bacteria. TPS systems secrete large, mostly beta-helical proteins called "TpsA" that serve as virulence factors. FhaC, the outer-membrane transporter that secretes the Bordetella pertussis adhesin filamentous haemagglutinin (FHA) is one of the most characterized TPS system. The structures of FhaC (1-4) and of FHA (5) have been determined, providing structural insights into this secretion process. The structural and functional data on the FhaC/FHA system will be presented. They allow to propose a model for transport of FHA across the outer membrane, which may apply more generally to the secretion of TpsA proteins by their dedicated TpsB transporters. In conclusion, we have determined the first crystal structure of a member of the Omp85-TpsB transporter superfamily. It offers molecular insights into how proteins get into and across cellular membranes.

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Keywords: bacterial membrane, protein transport, POTRA

KN32

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Crystal engineering of co-crystals and their relevance to pharmaceuticals and solid-state chemistry

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The field of crystal engineering has evolved in such a manner that it has become synonymous with synthesis of new classes of organic and metal-organic compounds. Crystal engineering invokes self-assembly of existing molecules or ions and therefore means that a wide range of new compounds can be generated without the need to invoke covalent bond breakage or formation. This presentation will address a long-known but little studied class of compound,

co-crystals, and it will highlight their relevance to pharmaceutical science and solid-state chemistry. The presentation will be organized as follows:
A general introduction to the when, how and why of co-crystals with emphasis upon the hierarchy of hydrogen bonds that can be exploited to design co-crystals from first principles;
Pharmaceuticals are perhaps the most valuable materials known to mankind and there are important intellectual property, regulatory and efficacy implications if one is able to discover new compositions of matter for active pharmaceutical ingredients (APIs). Emphasis will be placed upon pharmaceutical co-crystals, a long known but little explored alternative to more widely accepted forms of API such as polymorphs, solvates, salts;
The potential impact of co-crystals on green strategies for the synthesis/processing of fine chemicals such as APIs and novel ligands for nanoscale polyhedra and their networks will be discussed with emphasis upon co-crystal controlled solid-state synthesis (C3S3);
The use of co-crystals involving homochiral co-crystal formers for resolution of enantiomers will be discussed.

Keywords: hydrogen bonding, solid-state synthesis, pharmaceutical compounds

KN33

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Quasicrystals structures properties and applications

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Quasi-crystal (Qc) is no longer a unique structure matter since it has been confirmed as a equilibrium phase in more than one hundred alloys. It is clear that stability of stable Qcs can be understood within the frame work of Hume-Rothery rules. Even more interesting, it is found that stable Qcs are strict electron compounds, which only formed for alloys with sharp valence electron concentration (e/a: electron-atom ratio). Actually, most stable Qcs were discovered on the basis of the e/a criterion. With these stable Qcs, structural analysis is allowed to study on a single grain sample. Although few structural models have been proposed, they still suffered from considerable uncertainty due to topological and chemical disorder. Recently, understanding in structure has been highly improved in a binary Cd-Yb Qc. Furthermore, observed surface structures of quasicrystals by STM have been well interpreted by bulk structural model. This talk will mainly deal with three topics; the first one is the Hume-Rothery rules for stable Qcs, the second one is regarding the structure of a binary Cd-Yb Qc and the third one is the surface structures in relation to bulk structural models for Qcs.

Keywords: quasicrystals, stability, structures of inorganic compounds

KN34

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Focused structural genomics

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The genome sequence data allow comprehensive approaches to studies of complex cellular systems. Advances in structural biology have expanded our competence in determining protein structures. World-wide Structural Genomics efforts contributed a complementary array of rapid, integrated, cost effective methods and created efficient structure determination pipelines. The semi-automated pipeline of the Midwest Center for Structural Genomics (MCSG), one of the Large-scale Production Centers of the NIH-funded Protein Structure Initiative (PSI) has allowed the MCSG to determine over 800 structures that are annotated for function and ligand binding. Results, data and homology models are made available to the scientific community. The PSI has sampled the entire prokaryotic protein sequence space more broadly than ever before. Many protein families are of high biological and biomedical interest. Important trends have emerged from this research: very distant protein sequence families share the same fold and proteins with similar structures have evolved different functions. The PSI continues to contribute to an understanding of molecular mechanisms and plays a significant role in the discovery of the evolutionary, structural and functional relationships among protein families that are often not apparent from their sequences. This research provides a wealth of ideas, concepts and understanding of mechanisms for acquisition of novel biological function and the evolution of biological systems.
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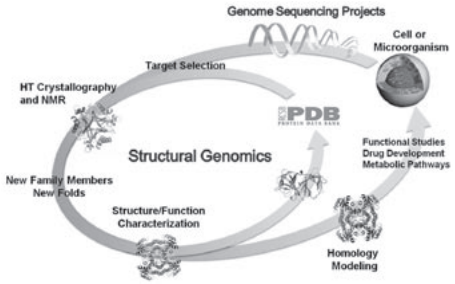

Keywords: structural genomics, protein families, protein evolution

KN35

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Science at XUV and hard X-ray free electron lasers

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In recent years modern storage ring based synchrotron radiation facilities have been very suc-cessful in enabling structure determination with atomic resolution on nanoscale samples. X-ray free electron lasers (FEL) at linear accelerators provide extremely intense, ultra-short pulses of coherent X-rays and allow direct access to system dynamics on the atomic time scale. In flashes of 10 femtoseconds duration FELs provide as many photons as we get today from the best stor-age ring facilities per second and therefore we can e.g. envisage to take movies of molecular machines at work instead of pictures of their time averaged structure. The broad and very com-pelling science case motivated the construction of 3 hard X-ray FELs: The Linac Coherent Light Source LCLS in Stanford, USA, which will start operation in summer 2009, the Spring-8 Com-pact SASE Source SCSS in Japan, which is expected to start operation in 2011, and the Euro-pean XFEL Facility in Hamburg, Germany, with start of operation expected for 2014/15. FLASH, the Free Electron Laser at DESY in Hamburg is the first X-ray FEL providing beam in the spectral range of the VUV and soft X-rays. It is operated as a user facility since summer 2005 and research is currently focused on understanding the interaction of extremely