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

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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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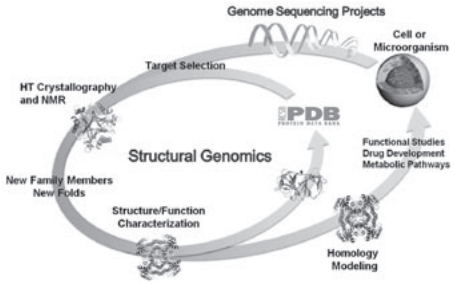

Keywords: structural genomics, protein families, protein evolution

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

intense X-ray pulses with matter. Some of the results obtained so far, including the first steps towards single particle imaging, will be presented. The FLASH results strongly support the high expectations for revolutionary science from hard X-ray FELs.

Keywords: synchrotron radiation, free electron lasers, ultrafast dynamics

KN36

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Structure refinement and structure modelling: A chemical probe for complex mineral groups

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Minerals usually show widespread solid-solution of many chemical species in a number of structural sites. In rock-forming minerals, cation site-preference and partitioning (when allowed by the crystal structure) depend on both bulk composition and system parameters such as pressure, temperature and water activity, so that cation ordering patterns provide important clues on the evolution of petrogenetic processes. Cation order in a given sample can be inferred by structure refinement (SREF) and supported by spectroscopic analysis; far more reliable results are obtained by comparison with crystal-chemical models based on many solid-solution terms. Surprisingly reliable results can also be obtained via statistical analysis of representative databases built up with a multi-analytical approach including SREF and in situ analysis of all the chemical constituents (H, Li, Be, B included, if relevant to the crystal-chemistry of the mineral group). In the case of the amphiboles, detection and quantification of even elusive constituents such as Li and the oxo component, as well as calculation of the crystal-chemical formula, can now be addressed based only on combination of subtle changes in the geometric and electronic descriptors derived from SREF. Also, reliable regression equations now relate the crystal-chemical formula with unit-cell parameters. They can be used to check the composition of small synthetic crystals (often off composition with respect to the reagents), where in situ analysis is impossible and the only available evidence is powder diffraction analysis. They also provide clues for the non-existence of some particular composition, among which many theoretical end-members. Examples will be given focussing on the crystal-chemistry of amphiboles and garnets.

Keywords: crystal structure databases, single-crystal structure analysis, mineral crystal-chemistry