specialists in order to investigate the structures of aperiodic crystals including incommensurately modulated crystals, composites and quasicrystals. Composite and modulated structures occur in almost every type of solids including organic and inorganic compounds, minerals, metals and alloys and even in proteins. The study of their structures has greatly contributed to identify and understand the interactions occurring in crystals. Numerous phenomena, which were partially understood, could be reinterpreted on the basis of the incommensurability of structures. The superspace formalism appears to be particularly suited for the description of modular structures, i.e. structures sharing common building units. This has been applied to a series of technologically important class of compounds including perovskites, ferrites and sheelites. In some favourable case, the full series of compounds can be described with a single parameter, characterising the chemical composition of each member. The presentation is intended to illustrate the evolution of the superspace concept since it was introduced some four decades ago.

Keywords: aperiodic crystallography, superspace symmetry, incommensurate structures

KN26

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Materials research with scanning microfocus small-angle X-ray scattering

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Complex materials are often inhomogeneous at many length scales. This is true, in particular, for biological materials, such as bone, wood, arthropod or mollusc shells. More generally, graded functional materials in biology or in engineering require special characterization techniques to account for the fact that the structure at the nanoscale varies spatially on the scale of microns or larger. Scanning micro- and nano-focus small-angle x-ray scattering offers a unique tool for obtaining structural information from the molecular to macroscopic length scales, combining the powers of scattering analysis with scanning imaging. The lecture reports recent progress focussing on examples from biology and materials science.

Keywords: SAXS, microfocus, hierarchical structure, biological meterials

KN27

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Using neutrons and synchrotron X-rays together: Looking at the full picture in condensed matter

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Neutrons and synchrotron xrays are truly complementary probes. The matrix elements for the scattering of neutrons are straightforward and diffraction and inelastic scattering provide quantitative information on magnetic and chemical structure. Hard xrays on the other hand can be considerably harder to interpret but provide very high wavevector accuracy and information on the electronic and magnetic states through resonant scattering. In the soft xray regime the matrix elements for charge and orbital scattering again can become simpler but with the challenges of limited wavevector ranges, surface effects, and the need to work under ultra high vacuum. In this talk I will present a few selected materials whose complex structure and behaviour is becoming clear by the coordinated use of multiprobe scattering techniques. From these examples areas of importance for the challenges of the future will be discussed.

Keywords: neutron and X-ray scattering, magnetic materials, transition metal-rare earth oxides & intermetallic

KN28

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Structural pharmacology and drug discovery: Exploring biological and chemical space

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Knowledge of the three-dimensional structures of protein targets that is now emerging from structural proteomics and targeted structural biology programmes has the potential to increase our understanding of human genetic variation, as well as to accelerate drug discovery. Protein structures provide insights into human genetic variation, including both non-synonymous single nucleotide polymorphisms and somatic mutations and their relationships to disease. This is exploring biological space. Structural analyses can also be used to explore chemical space, to investigate the chemical molecules that proteins might bind. This can be defined by fragment-screening techniques, which inform not only lead discovery but also optimization of candidate molecules. A range of biophysicaltechniques can be exploited, buthigh-throughput X-ray crystallography focused on identifying several weakly binding small-molecule fragments from compound libraries consisting of hundreds of small-molecule fragments has huge strengths and is an effective way of defining the chemical space of potential ligands. The high-resolution definition of these binding interactions provides information-rich starting points for medicinal chemistry. The use of high throughput X-ray crystallography does not end there, as it becomes a rapid technique to guide the elaboration of the fragments into larger molecular weight lead compounds. I will describe such developments not only in industry but also in academia for diseases of poverty, rare diseases and difficult targets. A long-term objective must be to define the chemical space around all macromolecules in man and in pathogens, so as not only to facilitate lead discovery but also to identify potential off-target interactions and minimise side effects.

Keywords: structural biology, drug discovery, design

KN29

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Metal-organic materials: Strategies toward functional porous materials

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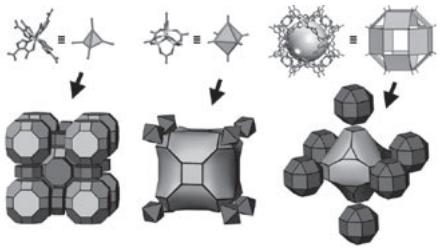
The quest for functional materials targeted for specific applications is ever increasing as societal needs and demands mount with advancing technology. One class of inorganic-organic hybrid materials, metal-organic materials (MOMs), has burgeoned in recent years due, in part, to effective design strategies (i.e. reticular chemistry) for their synthesis and their inherent [and readily interchangeable] hybrid,

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,