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,