

## KN25

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***E. coli* co-translational targeting complexes studied by cryo-EM**  
 Christiane Schaffitzel, *European Molecular Biology Laboratory, Grenoble (France)*. E-mail: schaffitzel@embl.fr

The signal recognition particle (SRP) and its receptor FtsY target nascent polypeptides containing a hydrophobic signal sequence to the translocation machinery in the inner membrane. The SRP and FtsY contain homologous GTPase domains which are an integral part of the targeting cycle. The structures of the *E. coli* SRP [1] and of the SRP-FtsY complex [2] bound to the translating ribosome have been solved by cryo-electron microscopy. The SRP-FtsY complex presents the *early*, nucleotide-independent conformation of the complex. The SRP is prepositioned for the binding of FtsY when bound to the ribosome nascent chain (RNC) complex. FtsY docks onto the RNC-SRP complex forming direct contacts with the SRP NG domain and the 4.5S RNA. The homologous NG domains of Ffh and FtsY interact weakly. The SRP RNA tetraloop contacts the FtsY GTPase domain and holds FtsY in place for interaction with the Ffh NG domain. This structure explains how the RNC stabilizes the SRP-FtsY complex in the *early* conformation, thereby delaying subsequent conformational rearrangements in the GTPase complex that lead to GTP hydrolysis and hand-over of the translating ribosome to the translocation machinery.

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**Keywords:** single particle electron microscopy, ribosome, signal recognition particle

## KN26

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**Topological variations in inorganic oxocompounds: origin of structural diversity**

Sergey V. Krivovichev, *Department of Crystallography, St. Petersburg State University, St. Petersburg, Russia*. E-mail: skrivovi@mail.ru

Inorganic oxocompounds display an outstanding structural diversity of structural topologies and compositions [1]. One of the main problems of crystal chemistry is to arrange known structural architectures into a coherent scheme of structural hierarchy with different levels of complexity and obvious topological interconnections between different classes of structures. Another crucial point, which is not experimentally easily accessible nowadays, but may become an important area of research in the future is the origin of structural diversity and complexity from the local molecular-scale interactions.

A number of mathematical techniques have been employed in order to describe topology of linkage of structural units in inorganic compounds, metal-organic compounds and polymers. These techniques include: networks, graphs and tilings, and all mathematical instruments associated with these concepts. A range of computational programs and databases have been developed in this field.

Using inorganic oxysalts as an example, we have demonstrated that most of the observed topologies can be derived from a small number of simple (basic or archetype) graphs [1]. However, by definition, the structure is thought to be infinite if we describe it in terms of infinite symmetry groups, whereas real crystals are always finite and periodic only in a small portion of space. The local interactions that lead to the formation of crystals can be described in terms of automata with each step of attachment of a molecular or atomic fragment corresponding

to the transition of automaton from one step to the other. Since the structure is (locally) periodic, its automaton contains a finite number of states, i.e. is a finite deterministic automaton. Topology of state diagram of the automaton indirectly corresponds to the topology of quotient graph that describes linkage between adjacent structural units. Introduction of automata theory allows to link structural topology to the theory of formal languages and grammars [2] and to define such concepts as topological complexity on the rigorous basis of the theory of computation. In fact, any crystal can now be considered as a result of a cyclic computational process, where the role of the computer is played by the growing structure and structure of its program is controlled by energetical and spatial constraints.

A particular class of automata is cellular automata [3], which can be used for description of growth of complex structural topologies [4, 5].

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**XAFS Contribution to Protein Structure-Function Investigations**

S. Samar Hasnain, *Molecular Biophysics Group, Faculty of Health & Life Sciences, University of Liverpool, UK*. Email: S.S.Hasnain@liv.ac.uk, [www.biophysics.liv.ac.uk](http://www.biophysics.liv.ac.uk)

Metalloproteins utilise the redox properties of their metal atom(s) to cycle an enzyme through different reaction states. The structural differences between these redox states can be small thus requiring very high and often even atomic resolution crystallographic structures to distinguish between them. The high intensity of X-rays available from the most advanced sources together with improvements in crystallisation and detectors is helping to achieve these very high resolutions but the increased brightness of beams is also resulting in X-ray induced radiolysis of the metal centres which act as a very efficient electron sink in view of their redox properties.

XAFS, which probes the metal centre and is capable of providing sub-atomic resolution as well as information on the electronic configuration of the site, has been playing a central role in improving the precision and very often in providing information which otherwise is inaccessible by Crystallography since the emergence of synchrotron radiation in the late 70's. More recently, it has been used in conjunction with protein crystallography in a variety of ways to provide new opportunities for investigating this particular class of proteins. In addition to the use of polarized nature of synchrotron X-rays for angular-resolved XANES of single crystal, it is playing an important role in acting as control for the oxidation state of the metal centres in a protein structure determination. Some recent results will be presented to highlight the complementarity of the two techniques.

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## Keynote Lectures

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### Keywords:

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### Structural Basis of Cell Regulatory Processes

Leemor Joshua Tor, E-mail: leemor@cshl.edu

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### High-pressure studies of molecular crystals

Elena Boldyreva<sup>ab</sup> <sup>a</sup>*Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk.* <sup>b</sup>*REC-008, Novosibirsk State University, Novosibirsk (Russia).* E-mail: eboldyreva@yahoo.com

During a long time high-pressure crystallography was dealing more with minerals, metals, and inorganic solids, which were interesting for physics, mineralogy, geochemistry, or materials sciences. Diffraction studies of the organic solids and coordination compounds were limited, although the pioneering work by Bridgeman, Vereschagin, Kabalkina, Fourme, Katrusiak, Allan and some other researchers can be referred to. An enormous progress in the instrumentation and software development for high-pressure research was achieved in the last one-two decades, and this has made diffraction studies possible even for low-symmetry organic crystals. Together with an increased interest in molecular crystals with respect to their applications as materials, devices and pharmaceuticals, this has resulted in a noticeable increase in the number of research groups involved in high-pressure diffraction studies of organic and coordination compounds. This lecture aims to give a general overview of the research in this field, in retrospect and prospect. Attention will be paid, in particular, to the following aspects of research: i) crystallization at high pressure; the crystal structures of high-pressure phases as a tool to study intermolecular interactions; ii) studies of the anisotropic structural strain within the limits of stability of the same phase; understanding the intermolecular interactions; iii) phase transitions at high pressure, thermodynamics and kinetics; iv) pressure-induced chemical reactions; v) effect of pressure on thermal / photochemical reactions.

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### Powder diffraction at the nanoscale: structure and defects

Reinhard B. Neder<sup>a</sup> <sup>a</sup>*Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen, Staudtstr. 3, 91058 Erlangen (Germany).* E-mail: reinhard.neder@krist.uni-erlangen.de

Powder diffraction pattern of nanostructured materials are characterized by broad maxima that overlap widely. This is accentuated if additional defects are present, which destroy the remaining periodicity of the object. Thus the information content that appears to be present is reduced and standard structure determination and refinement procedures do not work any longer. The shape and continuous intensity distribution of these maxima do hold, however, a lot of information on the particle size and defects, which can quantitatively be interpreted by appropriate whole pattern matching.

If the diffraction pattern is measured to very high values of  $Q$ , above some  $20 \text{ \AA}^{-1}$ , a lot of further information about the sample is collected, despite the fact that the diffraction pattern at high  $Q$  does not contain any sharp features but broad oscillations at best. With this high  $Q$  range, the powder pattern can be transformed via a sine Fourier