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***E. coli* co-translational targeting complexes studied by cryo-EM**
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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.

[1] Schaffitzel, C., Oswald, M., Berger, I., Ishikawa, T., Abrahams, J.P., Koerten, H.K., Koning, R.I. & Ban, N. *Nature* **2006**, *444*, 503-506.

[2] Estrozi, L.F., Boehringer, D., Shan, S.O., Ban, N. & Schaffitzel, C. *Nature Structural & Molecular Biology* **2011**, *18*, 88-90.

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Topological variations in inorganic oxocompounds: origin of structural diversity

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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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[1] S.V. Krivovichev, *Structural Crystallography of Inorganic Oxysalts*, Oxford University Press, Oxford, **2009**. [2] N. Chomsky. *Syntactic Structures*, The Hague: Mouton, **1957**. [3] S. Wolfram, *A New Kind of Science*, Wolfram Inc., **2002**. [4] S.V. Krivovichev, *Acta Crystallogr.* **2004**, *A60*, 257. [5] S.V. Krivovichev, *Eur. J. Inorg. Chem.* **2010**, 2594.

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XAFS Contribution to Protein Structure-Function Investigations

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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.

[1] I. M. F. Perutz, S. S. Hasnain, P. J. Duke, J. L. Sessler, & J. E. Hahn, *Stereochemistry of iron in deoxyhaemoglobin*, *Nature*, **1982**, *295*, 535-538. [2] P. Durham, A. Bianconi, A. Congiu-Castellano, A. Giovannelli, S. S. Hasnain, L. Incoccia, S. Morante & J. B. Pendry *The EMBO Journal*, **1983**, *2*, 1441-1443. [3] A. Bianconi, A. Congiu-Castellano, P. J. Durham, S. S. Hasnain &