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A Theoretician's View of Crystallography
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Whether thinking qualitatively or quantitatively, molecular structure, most often determined by crystallography, is central to the aims of quantum chemists. This long-time consumer and observer of crystal structures will talk about the conceptual terrain between theorists and crystallographers. Among the topics broached will be the complex problem of what is a chemical bond, experimental and "chemical" standard deviations, and the working out of secondary, donor-acceptor interactions in the solid state.
Keywords: molecular structure, secondary interactions, chemical bond

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Structure and Recognition in the BARS/CtBP-dependent Transcription Regulation
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BARS/CtBP3 is a dual function protein acting as acyl-transferase in the Golgi apparatus (supporting membrane reshaping and vesicle traffic) [1], and as transcription co-repressor, in the nucleus, through the interaction with several enzymatic partners (e.g. histone deacetylases, HDACs). BARS/CtBP3 is based on a 3-domain structure, hosting a classical dehydrogenase fold [2]. Regulation of the two activities is achieved through competitive binding of NAD(H)/acyl-CoA, association equilibria, SUMO-ylation, and eventually through recognition of specific sequence motifs in the interacting partners. Binding of specific transcription factors to each subunit in the dimeric BARS/CtBP3, through a PXDLS sequence motif, is considered one of the basic mechanisms to recruit HDACs, and modify the chromatin structure, with ensuing transcription repression [2]. Structural considerations and mutant analyses indicate that different recognition sites are present on BARS/CtBP3 surface, in keeping with its pivotal role within a nuclear protein complex hosting more than twenty different proteins.

[1] Weigert R., Silletta M.G., Spano S., Turacchio G., Cericola C., Colanzi A., Senatore S., Mancini R., Polishchuk E.V., Salmona M., Facchiano F., Burger K.N.J., Mironov A., Luini A., Corda D., *Nature*, 1999, **402**, 429. [2] Nardini M., Spano S., Pericola C. Pesce A., Massaro A., Millo E., Luini A., Corda D., Bolognesi M., *EMBO J*., 2003, **22**, 3122.
Keywords: biomolecular recognition, enzyme function, transcription regulation

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Ion Pumping by Ca^{2+}-ATPase of Sarcoplasmic Reticulum
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Ca^{2+}-ATPase of skeletal muscle sarcoplasmic reticulum (SERCA1a) is an integral membrane protein of 110K and the best characterised member of the P-type (or E1/E2-type) ion translocating ATPases. It transports 2 Ca^{2+} and counter-transports 2~3 H^+ per ATP hydrolysed. SERCA1a consists of 10 transmembrane helices, 3 cytoplasmic domains (A, actuator; N, nucleotide binding; P, phosphorylation) and small lumenal loops [1]. In E1, transmembrane Ca^{2+}-binding sites have high affinity and face the cytoplasm; in E2, the binding sites have low affinity and face the lumen of sarcoplasmic reticulum (extracellular side). Actual transfer of bound Ca^{2+} is thought to take place between E1P and E2P. We have determined the crystal structures of this enzyme in 5 different states [2], namely, Ca^{2+}-bound E1·2Ca^{2+}, Ca^{2+}-unbound but thapsigargin bound E2(TG), Ca^{2+}- and AMPPCP-bound E1·AMPPCP, Ca^{2+}-, ADP- and AlF_x bound E1·AlF_x·ADP, and Ca^{2+}-unbound but MgF_4^{2-} bound E2·MgF_4^{2-}, where MgF_4^{2-} and AlF_x work as stable analogues of phosphate. Detailed comparisons of these structures show that very large rearrangements of cytoplasmic domains and transmembrane helices take place, and that ATP, phosphate, Ca^{2+} and Mg^{2+} are the principal modifiers of the domain interactions.

[1] Toyoshima C., Inesi G., *Ann. Rev. Biochem*., 2004, **73**, 269. [2] Toyoshima C., Nomura H., Tsuda T., *Nature*, 2004, **432**, 361.
Keywords: ion pump, membrane proteins, inhibitors

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Neutrons and X-rays for Microstructure and Strain/Stress Analysis in Materials
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The microstructure and the strain/stress distribution in engineering materials can be adjusted as a function of the materials processing technology and its parameters. Since the microstructure and the strain/stress distribution in components are responsible for macroscopical properties, e.g. yield strength fatigue life, the property profile of components can be optimised in view of the in-service condition. The optimation requires the detailed knowledge about microstructural parameters like phase composition, grain sizes, dislocation densities, texture, strains/stresses and their relationship to the macroscopical properties. The various contributions to this field using X-ray and neutron diffraction are presented. Special emphasis is put to the rapid development of the microstructural and strain/stress analysis due to the increasing use of synchrotron X-radiation which enables new measuring techniques but also in-situ analysis of microstructural alterations and strain/stress developments. Examples are given for selected material systems like Mg-alloys and brass alloys.
Keywords: strain/stress, X-ray diffraction, Mg-alloy

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Single-particle Diffraction
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X-ray crystallography is approaching the time when it will be able to image single small objects without the need to aggregate multiple copies into a crystal. The emerging technique is quite close to that of x-ray crystallography, but replaces the crystal's large amplification of the diffracted signal by the use of high-intensity x-ray sources and techniques for minimizing the effects of radiation damage. The subject will be illustrated by describing progress in our project aiming at 3D 10nm-resolution imaging of a single quick-frozen yeast cell.

The talk will serve as an introduction to Microsymposium MS22, which will describe additional ongoing work, including projects aimed at atomic-resolution imaging of single macromolecules and macromolecular assemblies by the use of femtosecond-length pulsed x-ray sources.
Keywords: crystallography without crystals, X-ray diffraction microscopy, yeast cell

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Elucidating the Structures of Nanoporous Microcrystals
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With their stable and open aluminosilicate framework structures, zeolites and their analogs have proven to be ideally suited for intriguingly diverse applications. Their pore openings, which range from 0.25 to 2.0 nm, have molecular diemensions; their void space can reach up to 50% of the total volume; they are crystalline with well-defined and ordered pores; and their framework structures are anionic or neutral. These features are exploited in their use as