KN01

Conformational Change and Assembly of Proteins into Amyloid fibrils Elisabeth Sauer-Eriksson[a], Anders Karlsson, Anders Olofsson, Malin Lindhagen-Persson, Anders Öhman *Umeå Centre for Molecular Pathogenesis, Umeå University, Sweden.* E-mail: liz@ucmp.umu.se

Keywords: amyloid, conformational change, protein structure

Self-assembly and deposition of proteins into amyloid fibrils and plaques have currently been linked to around 20 different human diseases. The best known examples of such disorders are Alzheimer's disease and prion diseases. Amyloid contains extremely insoluble protein fibrils (50-150 Å) that share similar morphological features but comprise many different proteins with no obvious sequence similarity. Amyloid formation and deposition are complex processes yet to be fully understood. Evidence from numerous in vitro studies shows that amyloid formation is a multistep process involving amyloidogenic intermediates. Structural and biophysical studies on amyloid-forming proteins are pursued with the aim to elucidate further information about the structural composition of amyloid and amyloid-forming intermediates. In this talk I will review some of our work with reference to three amyloidogenic proteins: amyloid-β-peptide, medin, and transthyretin.

KN02

Software for the refinement of aperiodic and incommensurate structures Václav Petříček[a], Michal Dušek[a], Lukáš Palatinus[ab], [a]*Institute of Physics, Praha, Czech Republic,* [b]*Ecole Polytechnique Fédérale de Lausanne, Laboratoire de Cristallographie, Lausanne, Switzerland* E-mail: petricek@fzu.cz

Keywords: modulated crystal structures, structure analysis, superspace theory

The refinement of modulated structures requires a specific modification of traditional refinement programs to account for additional satellite reflections. The most natural and effective way is application of the superspace theory developed by DeWolff, Jansen & Janner [1] which makes possible to apply symmetry and generalize all formulas for calculation of structure factors. Then modulated structures are described by the same set of parameters (atomic occupancies, coordinates and displacement parameters) but they can are now a periodic functions of the actual position of atom in the crystal. This new periodicity can be generally incommensurate with the basic translation periodicity. The basic ideas and several examples of application will be presented in the first part of the lecture. Modulation functions for occupancy in many cases have non-continuous character. Then a special function called *crenel* is to be used [2]. A new numerical method, based on using orthogonalized polynomials enhancing stability of the refinement, has been recently included into the new JANA2006. Typical examples will document main advantages of this approach.

The program Superflip written by L.Palatinus, based on the new progressive method for solution of modulated structures *charge flipping* [3], prove to be the best way how to solve even strongly modulated structures. Jana2006 allows applying of this method by direct calling of the Superflip.
The new Jana2006 can also be used for refining of magnetic structures. It can be applied even for combination of nuclear and magnetic modulations in the crystal.
The last new option in Jana2006 is possibility to combine data from different sources. Several sets of powder data and single crystal data from neutron and X-ray diffraction can be refined simultaneously.

[1] Wolff de P.M.; Janssen T; Janner A. *Acta Cryst.* A37, (1981), 625.
[2] Petříček, V.; van der Lee; A. & Evain, M. (1995). *Acta Cryst.* A51, 529.
[3] Palatinus L. *Acta Cryst.* (2004). A60, 604.

KN03

Cutting and Moving DNA Miquel Coll, *Institut de Recerca Biomèdica & Institut de Biologia Molecular (CSIC), Josep Samitier 1-5, Barcelona, Spain.*
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Keywords: Protein-DNA complexes, DNA translocation, Bacterial conjugation, Horizontal gene transfer

Mechanisms of horizontal gene transfer in bacteria are typically categorized into transduction, transformation and conjugation. Transduction is mediated by bacteriophages, which may incorporate fragments of the host bacterial DNA and transfer them into the infected hosts. Natural transformation consists in the uptake of portions of naked DNA. Finally, conjugation is the unidirectional transfer of single-stranded plasmidic DNA from a donor bacterium cell to a recipient cell. Conjugation endows bacteria with a mechanism for the rapid acquisition of new genetic information. Rampant antibiotic resistance among pathogens is a troubling consequence of this microbial capacity. DNA transfer across cell membranes requires sophisticated machinery formed by a number of proteins that first perform the DNA processing and then its transmembrane transport. Although bacterial conjugation was discovered in the 40s, only now are we unveiling the molecular mechanisms behind it. In particular, structural biology [1] is providing a detailed view of the molecular architecture of several of the pieces involved, showing their evolutionary relationship with DNA replication and protein transport systems.

[1] Gomis-Rüth, F.X. & Coll, M. (2006) Cut and Move: Protein Machinery for DNA Processing in Bacterial Conjugation. *Curr. Op. Str. Biol.* 16, 744-52.

KN04

Hydrophobic dipeptides as building blocks for the construction of nanoporous organic materials Carl Henrik Görbitz, *Department of Chemistry, University of Oslo, Norway.* E-mail: c.h.gorbitz@kjemi.uio.no

Keywords: dipeptides, microporous materials, supramolecular chemistry

In the last few years dipeptides with two hydrophobic residues (hydrophobic dipeptides) have emerged as an unexpected source of stable microporous organic materials. Supramolecular self-assembly of the rather

small building blocks is dictated by stringent demands on the hydrogen bond formation by the peptide main chains and the aggregation of hydrophobic entities in the side chains. Some of these peptides have a marked propensity for cocrystallization, thus forming layered crystal structures as inclusion compounds with peptide hosts and various simple organic molecules as guests. A systematic survey of structures derived from single crystal X-ray diffraction studies has furthermore revealed the existence of two large classes of nanotubular micropourous structures, differing in the dimensionality of the hydrogen bonding patterns in the crystals and the nature of the channels. The lecture gives an overview of the structural aspects of the hydrophobic dipeptides and discusses the potential applications of these remarkable organic materials.[1]

[1] Görbitz, C. H., *Chem. Eur. J.* 2007, 13, 1022-1031.

KN05

Crystallography in Art and Archaeology Eric Dooryhee, *Institut Neel, CNRS Grenoble, France*
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Keywords: symmetry, applied crystallography, work of art

The regular, and sometimes particularly complex, inner arrangement of atoms and molecules in a crystal has always had a naturally artistic appearance. It is undeniable that subdivisions of the 2D or 3D space based on crystal-like shapes, repeated patterns, symmetry groups and crystallographic rules have been and still are a source of profound inspiration for many artists. Symmetry, or the lack of symmetry, has been a central concept in science since ancient times, and prevail in various fields of art: painting, sculpture, architecture, music, dance, poetry... In the first part of the talk, various examples and illustrations will show how the formal qualities of a work of art intersects the basics of crystallography.
Symmetry is often assimilated to the idea of harmony, based on a rational and clear principle of organization and order. The concepts of symmetry convey a charming impression and sometimes provide the artist with appropriate solutions. They produce a pleasant balance between our senses and our thought, enhance our perceptions of harmony and contribute into higher understanding and emotions in front of a master piece. Crystallography and crystal physics provide a cognitive basis for deriving the descriptive morphological and structural classifications of natural objects, and their real or imaginary analogues in art and archaeology.
The diffraction techniques reveal the regular arrangement of the atoms and molecules in an orderly solid. Crystallographic modelling shows the symmetry rules underlying this assembly. Many crystallographic representations (such as ball-and-stick models or measured electron density maps) can be considered themselves as artistic and symbolic views of the reality. Some of them closely resemble a scaffold, which gives us a feeling for the representation of infinity but which may also appear like a dead body without a soul. Only after putting back the fundamental motifs (the atoms, the molecules, or any man-made form) does the fascination for symmetry plainly appear again.
The last part of this talk discusses the recent implementation of crystallographic methods while addressing some enigmas in the fields of archaeology and art: the identification and provenance of the materials, the trading routes, the elaboration procedures and the artists' know-how, the authentication, the transformation and preservation of the artefact with time. The history of these objects, as part of our cultural heritage, is often embedded in the structure and micro structure of the component materials, and needs to be deciphered every time ancient texts are silent or absent.

KN06

Dynamic Electron density: a unique link between advanced X-Ray experiments and reactivity [a]Pierre Becker, [b]Nour Eddine Ghermani, [a]Jean Michel Gillet, [a]Blandine Courcot, *a*: *Ecole Centrale Paris, Laboratoire SPMS, Grande Voie des Vignes, 92295 Chatenay Malabry Cedex, France – b: Faculty of Pharmacy, University Paris XI, 92295 Chatenay Malabry Cedex, France*
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Keywords: electron density, high resolution scattering, time resolved scattering, microscopic time evolution of matter.

Charge, spin and momentum density studies lead to a challenging interplay between experimental and theoretical viewpoints concerning binding and cohesive effects in condensed matter. Recent achievements concerning pharmaceutical or biological systems allowed for a critical estimate of the level of transferability of charge density, with an important impact towards modelling physico-chemical mechanisms in those complex media.
Charge density indeed plays a crucial role, owing to its leading character in the description of the electronic ground state of any system. Though most studies have focused on one type of density, it is clear that the three density components are linked through the reduced one particle density matrix (1RDM). Through combined studies of momentum and charge density, we have been able, in our group, to show that the 1RDM in a solid can be developed as a sum of fragment contributions: each of them incorporates interactions with neighbouring fragments through finite clusters ("cluster partitioning method"). It is thus possible to overpass the strict periodicity condition and to consider systems that are disordered or undergoing structural changes. This method will be discussed, focussing towards modelling of a given fragment in variable environments. It has recently been possible to extend this approach to pharmaceutical molecules and to reach the key question of their activity within biological medium.
Recent experimental developments have opened a revolutionary path combining X Rays and neutrons with laser pulses. Charge and spin density in photo-excited solids have led to crucial observation of electronic behaviour in non equilibrium states of condensed matter. The fast development of time resolved X Ray scattering allows for the observation and microscopic modelling of systems undergoing chemical reactions, phase transitions, response to applied actions. The key function associated to such mechanisms is the time dependent charge density $\rho(\mathbf{r},t)$ and its generalisation to time dependent 1RDM. We shall discuss the present status of time dependent scattering, together with some tentative modelling. For a system undergoing a chemical reaction, one must identify the reaction path, through the Fukui intrinsic reaction