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

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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

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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 $\rho(\boldsymbol{r},t)$ 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