the Mirador de Lindaraja in the Alhambra and line the walls of the Patio de las Doncellas in the Alcázar, with further examples in the mosque of Cordoba, whereas the adverse fate relegated the ingenious decagonal Granada pattern to the Museum of the Alhambra. The artisans of the 14th century created further geometric, highly ornamental variations of octagonal, originally quasiperiodic mosaics which enliven the walls of the Tower of Comares and Torre de la Infanta in the Alhambra.

Keywords: Hispano-Islamic art, Alhambra, quasiperiodic patterns

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Charge densities and materials crystallography

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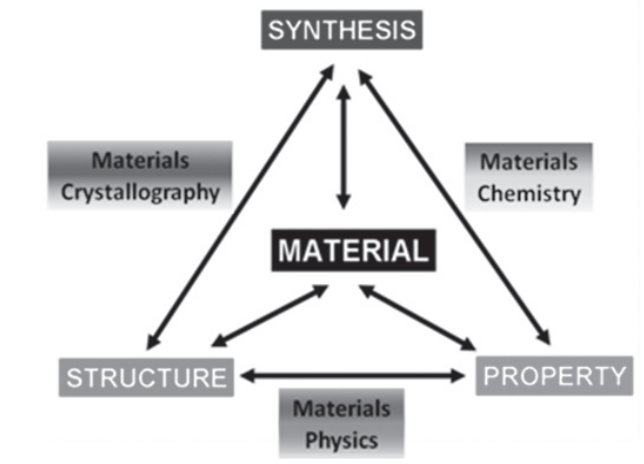
The Center for Materials Crystallography (CMC) is a new Center of Excellence funded by the Danish National Research Foundation with participating partners from Aarhus University, Universität Göttingen, University of Western Australia, Istituto di Scienze e Tecnologie Molecolari in Milano, the Advanced Photon Source, SPring8-RIKEN and Oak Ridge National Laboratory. CMC has focus on fundamental materials research, where strong competences in synthesis, characterization, and theoretical modeling are combined to tackle important challenges in materials science. The center has a broad range of activities including photocrystallography, molecular self assembly and host-guest interaction, complex magnets, nanoporous materials, in-situ studies, high pressure studies, thermoelectric materials and development of new crystallographic tools. Knowledge of the 3D structure of molecules, nano-particles and crystals is the key point for understanding, designing and manipulating chemical behavior or physical properties of materials. However, in more and more of the CMC studies it is becoming possible to move beyond the independent atom approximation of conventional structural crystallography, and determine the full charge density distribution in the crystals. The talk will discuss CMC charge density studies of thermoelectric materials, organic host – guest complexes, hypervalent materials, metal organic framework materials and polynuclear transition metal complexes. Furthermore, recent development of multipole modeling of synchrotron powder diffraction data will be addressed.



Keywords: materials crystallography, electron density, nuclear density

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The SHELX approach to experimental phasing of macromolecules

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The programs SHELXC/D/E [1] for the experimental phasing of macromolecules are designed to be fast and easy to use (for both humans and GUIs such as hkl2map [2]), but achieve their robustness and speed by making some major simplifications. It is assumed that only one type of heavy atom or anomalous scatterer is present, so it is not necessary to specify *f'* and *f"* values. The initial native phase ϕ_{nat} is calculated as $\phi_{ha}+\alpha$, where ϕ_{ha} is the phase of the heavy-atom substructure. The heavy atoms are found by integrated Patterson and direct methods from the estimated heavy atom structure factor F_A. F_A and α are derived directly from the experimental data; for example for SAD phasing F_A is approximated by $|F_{hkl}-F_{-h-k-l}|$ and α by 90° when $F_{hkl} > F_{-h-k-l}$ and by 270° when the opposite is true.

The resulting electron density is improved by the *sphere of influence algorithm* [3] to make it more like the expected density without needing to define a solvent boundary. In the latest beta-test version of SHELXE, a poly-Ala trace is recycled to improve the phases for the next round of density modification [1]. This makes it possible to bootstrap from very weak starting phase information to a relatively complete backbone trace and a high quality map, especially when the native data extend to a resolution of 2.5 Å or better. The map quality can be improved further by extrapolating the data to a higher resolution than could actually be measured (the *free lunch algorithm* [4], [5], [6]).

A molecular replacement (MR) solution can also provide starting phases for the SHELXE density modification, which has the advantage of reducing the model bias associated with MR. When anomalous signal is available but is too weak for the direct location of the heavy atoms using SHELXD [7], such density modified MR phases ϕ_{mr} may be used to calculate an 'anomalous' map, with amplitudes F_A and phases $\phi_{mr}-\alpha$, to obtain the positions of the anomalous scatterers. This MRSAD approach [8] enables correct MR solutions to be identified and provides additional phase information that can be used either with or without the MR phases for further iterative density modification and poly-Ala tracing with SHELXE.

The ability of the integrated density modification and poly-Ala tracing in SHELXE to bootstrap from a rather small percentage of the total scattering power is exploited by ARCIMBOLDO, [9] which feeds a large number of possible MR solutions for small fragments such as α-helices into SHELXE. If one is lucky, one or more of these trials, not necessarily those with the best MR figures of merit, lead to a complete trace. This is effectively an *ab initio* method for the solution of protein structures; all it currently requires is native data to 2 Å resolution or better, the presence of one or more α-helices and a powerful computer cluster!

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Keywords: SHELX, phasing, algorithms