KN18

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Atomic-resolution Real-space Imaging and Aberration Corrected Electron Microscopy

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The successful correction of lens aberrations has greatly advanced the ability of the scanning transmission electron microscope (STEM) to provide direct, real space imaging at atomic resolution [1]. Very complementary to reciprocal space methods, it is especially advantageous for aperiodic systems, nanostructures, interfaces and point defects.

Al-Co-Ni decagonal quasicrystals provide an excellent illustration of both the benefit of aberration correction in allowing light atom columns to be seen clearly, and in the power of the direct image to reveal broken symmetry within the 2-nm clusters, the origin of the quasiperiodic real space tiling [2].

Nanocrystals exhibit structures and properties with no relation to the bulk, for example the room-temperature catalytic activity of nanosized Au or the white-light emission from nanosized CdSe. Real space imaging combined with density functional calculations can unravel the origin of such surprising properties.

Aberration corrected STEM images can provide (projected) atomic coordinates with precision of a few pm. While not comparable to that achievable with reciprocal space methods, real-space imaging can provide such data unit cell by unit cell across an interface. Examples will be shown of $BiFeO_3$, mapping polarization and lattice parameter direct from a Z-contrast image, mapping octahedral rotations across interfaces with electrodes and finding evidence for interfacial charge [3]. EELS also can provide independent indication of interfacial charge transfer, and examples will be presented from complex oxide heterostructures illustrating how the origin of interfacial conductivity can be revealed [4].

The aberration-corrected STEM can also be used to provide depth resolution. Although not at the atomic level, the interior of a Si nanowire can be imaged free from any surface influence, and several Au point defect configurations have been revealed [7].

Finally, the direct imaging and identification of point defects in monolayer BN [8] and graphene will be presented, including the observation of local changes in dielectric function through single atom EELS.

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KN19

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Life at the single molecule level

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In a living cell, gene expression—the transcription of DNA to messenger RNA followed by translation to protein—occurs stochastically, as a consequence of the low copy number of DNA and mRNA molecules involved. Can one monitor these processes in a living cell in real time? How do cells with identical genes exhibit different phenotypes? Recent advances in single-molecule imaging in living cells allow these questions to be answered at the molecular level in a quantitative manner [1-4]. It was found that low probability events of single molecules can have important biological consequences [5].

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Keywords: single molecule, gene expression, imaging

KN20

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From plane groups to quasilattices: Hispano-Islamic art of the Alhambra, Cordoba and Sevilla

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The palaces of the Alhambra in Granada, the Royal Alcázar of Sevilla and the Great Mosque of Cordoba are treasures of Hispano-Islamic art, spanning several centuries, since about 780 to post-reconquest times of so-called Mudéjar art. The non-representative ornamental art applied to adorn this architecture developed over time from plane group-based ornaments through the interlaced and/or dichroic as well as polychromatic versions to intricate octagonal and decagonal quasilattices. The colourful brick-and-marble ornaments of Cordoba astonish us primarily by the intricate pattern-construction methods. The fact that 80% of the plane group patterns (especially the mosaics) in the Alhambra belong to *p*4*gm*, *cm* and *cmm* does not detract at all from their large variety and beauty. As elsewhere in the Islamic world, interlacing of the original mesh boundaries was frequently applied, either imaginary on the walls and in the mosaics or real, in openwork trellis. Layer groups must be applied to these patterns so that, for example, the familiar *p6mm* becomes *p*622 on interlacing. Another form of interlacing are the modular wooden ceilings in the Alhambra and the white quasiperiodic lattices in the Alhambra and Sevilla. About one half of the magnificent stucco ornaments on the walls and tympana of the patios of the Alhambra are interlaced, most often as interlacing of two different motifs, each with its own layer symmetry, e.g. the interlaced arch pattern *p*2*an* can be combined with the filling pattern which has *cm* or *p*211 as the plane/layer group of symmetry.

Dichroic mosaics were favoured by the Islamic artisans and they served as a basis for their special ways of constructing polychromatic patterns. One of them was to leave the white tile subset of the dichroic stage untouched and apply a colour modulation wave only to the black tile subset. Similar was the application of a concept of 'colour supertiles' to the latter subset, often as if interference of colour waves from two directions. The most sophisticated approach created what we can call 'sequentially dichroic patterns', when a new dichroic colouring was applied to the 'black' subset of the previous dichroic stage; this could be repeated several times. Perfect colouring as we know it was not used, the shimmering white subset appears to have been essential.

Creation of quasiperiodic octagonal and decagonal mosaic patterns in the 14th century can be considered as pinnacles of the Hispano-Islamic ornamental art. In these colourful cartwheel patterns, white interlacing describes Ammann-type quasilattices, with quasiperiodic sequences of unit and $\sqrt{2}$ intervals in the octagonal case and similar sequences of unit and τ (i.e., $(1+\sqrt{5})/2$) intervals in the decagonal case. The rosette- and star-studded quasiperiodic octagonal patterns adorn

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

KN21

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Charge densities and materials crystallography

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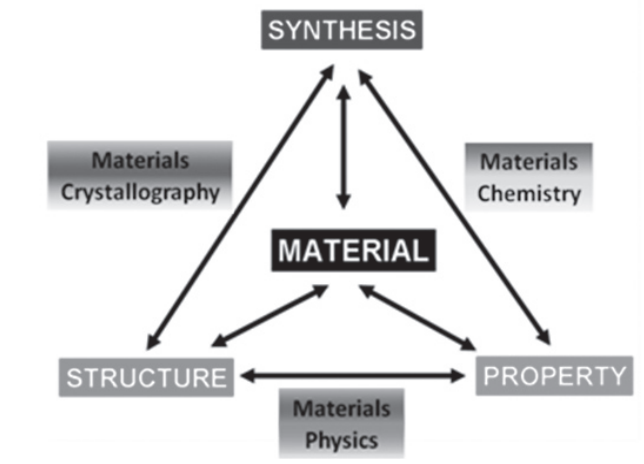
The Center for Materials Crystallography (CMC) is a new Center of Excellence funded by the Danish National Research Foundation with participating partners from Aarhus University, Universität Göttingen, University of Western Australia, Istituto di Scienze e Tecnologie Molecolari in Milano, the Advanced 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

KN22

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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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