(i) The theoretical developments made to analyse quantitatively the GISAXS patterns beyond the classical approximations, in particular to account for the profile of refraction index and the particle-particle correlations.
(ii) The self similarity during the dynamic coalescence of Au/TiO2(110) on the size distribution but also on the spatial ordering of the particles and its link with the randomness of the nucleation centers.
(iii) The sintering of nanoparticles during the course of the CO oxidation reaction and the link between particle size and chemical reactivity measured by mass spectrometry.

Keywords: GISAXS, growth, catalysis

## MS.03.1

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### Reliable determination of absolute structure using small Bijvoet differences

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Hooft et al. 2008 [1] contains a list of 11 data sets with MoKa radiation and 15 data sets with CuKa radiation that have been used to determine the absolute structure of the measured crystals using maximum likelihood and Bayesian statistics. The results compare favorable with the determination of the Flack x parameter [2] in that comparable standard uncertainties have been reduced by a factor of ~2. Since the submission of that paper additional experience was gained with the reliability of the absolute structure determination and the interpretation of associated statistics like the Normal Probability Plot [3] of the Bijvoet differences. We will address this experience and discuss small changes to the method that will further increase the robustness of the results.
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Keywords: absolute configuration, pharmaceutical compounds, maximum likelihood

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### Small molecule toolbox

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The Computational Crystallography Toolbox (cctbx)[1] provides a solid and comprehensive set of building blocks from which to construct crystallographic programs. Its core crystallographic library, which gave its name to the whole toolbox, is the foundation of the MacroMolecular Toolbox (mmtbx) which is the open source protein-specific component of the PHENIX system [2]. A sister library of the mmtbx, the Small Molecule Toolbox (smtbx), built on the top of the cctbx and addressing the specific need of small molecule single crystal solution and refinement is now under development. Ultimately we aim at writing the code necessary to give the practising crystallographer the tools (s)he is used to. Our focus is mainly on refinement and we will give a synthetic view of our implementation of F^2 refinement, weighting schemes, special position constraints [3], constrained Hydrogen atoms, constrained occupancies and ADP's for disordered atoms. We have also an interest in ab-initio structure determination and so far have coded the charge flipping algorithm. We will also discuss the problems raised by and the advances made in handling anisotropic scattering form factors, which are the key components for charge density refinement.
We gratefully acknowledge the financial support of EPSRC under grant number EP/C536274/1.
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[2] PHENIX: building new software for automated crystallographic structure determination, P.D. Adams, R.W. Grosse-Kunstleve, L.-W. Hung, T.R. Ioerger, A.J. McCoy, N.W. Moriarty, R.J. Read, J.C. Sacchettini, N.K. Sauter and T.C. Terwilliger. Acta Cryst. D58, 1948-1954 (2002) (http://www.phenix-online.org)
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Keywords: cctbx, small molecule, single crystal

## MS.03.3

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### The charge-flipping algorithm and related dual-space structure solution methods

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The dual-space iterative structure solution methods face an increasing interest among crystallographers, especially after the publication of the charge-flipping algorithm in 2004 [1], and demonstration of its usefulness for realistic crystallographic problems [2,3,4]. However, the history of the applications of the dual-space iterative algorithms for structure solution dates back at least to 1992, when the "low density elimination" method was published [5]. In 2003 a rather general algorithm named Difference Map was published [6]. It can be shown that all these algorithms can be described in a unified way using the language of constraint sets and projections. A constraint set is a set of all images (for example electron density) that fulfill a predefined constraint, for example positivity. A projection is then a mapping that maps any image onto an image in the constraint set. The different algorithms can be described as an iterative application of different combinations of two projections on a starting random image. It turns out, however, that not only the exact choice of the combination of projections is essential for the performance of the algorithm, but also the exact definition of the projections, constraint sets, and image play a crucial role. These settings distinguish the different algorithms that are otherwise conceptually related.
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