



YOUNG CRYSTALLOGRAPHERS SATELLITE MEETING

Monday 16th April

1.00-3.00 pm YC Session 1

YC Chemical Plenary

Speaker: Kenneth Shankland (Reading)

*Downhill all the way: an optimisation view of
crystal structures from powders*

3.30-5.00 pm YC Session 2

YC Biological Plenary

Speaker: Robin Owen (Diamond Light
Source)

*Seeing the full picture: combining
crystallography with tomography and
spectroscopy at I24*

5.30-7.00 pm YC Session 3

YCG AGM

Poster flash presentations

7.00-9.00 pm **Poster Session** with dinner and
wine

Tuesday 17th April

9.00-10.30 am YC Session 4

Parkin Lecture

Nominations should be sent to Anna Warren
(YCG Secretary/Treasurer)

10.30-11.15 am YC Session 5

Science Outreach



MEETING HIGHLIGHTS

Tuesday 17th April

12.15-1.00 pm **BSG Plenary**

Chair: Elspeth Garman

Speaker: Laurence Pearl (Sussex)

Title: TBC

Wednesday 18th April

9.00-9.45 am **The BCA Prize Lecture**

in honour of Dr Frank Allen

Speaker: Dr Robin Taylor (Taylor
Cheminformatics Software)

5.15-6.00 pm **IG Plenary**

Chair: Judith Shackleton

Dan Shechtman (Technion, Haifa, Israel and ISU,
Ames, Iowa, USA)

Quasi-Periodic Materials – Crystals Redefined

Thursday 19th April

9.00-9.45 am **PCG Plenary**

Chair: Ivana Evans

Branton Campbell (Brigham Young University)

*Symmetry modes: Nature's favoured
description of structural distortions*

Wednesday 18th April

10.00-11.45 am **Young Scientist Award
Ceremony**

Award of CCG CCDC Young Scientist Prize,
the Physical Crystallography Prize and the
Young Crystallographers Industrial Group
Prize Lecture will be announced and presented
at the meeting.

SCIENTIFIC PROGRAMME

Tuesday 17th April

1.30-3.00 pm Session 1

Multidimensional Materials

(Joint PCG and CCG Session)

This session will cover the use of crystallographic and imaging methods to understand the structure and properties of low-dimensional materials: zero-dimensional clusters, nanotubes, layered materials and frameworks.

Chair: Andrew Goodwin

Mark Weller (Southampton)

Valeria Nicolosi (Oxford)

Jeremy Sloan (Warwick)

Proteases in Disease

(BSG Session)

The session is themed around protease structure, mechanisms of proteolysis and understanding the regulation of complex processes such as blood coagulation and innate immunity.

Chair: James Huntington

Wilmos Fulop (Warwick)

*Oligopeptidases in peptide processing
memory disorders and pathogen virulence*

Piet Gros (Utrecht, Netherlands)

Proteases in complement and innate immunity

James Huntington (Cambridge)

Thrombin structure and dynamics

3.30-5 pm Session 2

Piecing Together the Puzzle – Multidimensional Approaches

(Joint CCG, YCG and PCG Session)

This session will cover investigations where a number of techniques are required in order to see the full picture. Sometimes we are so focussed on diffraction that we fail to see the added value of viewing the problem from a different angle. This session will show the benefits and extra information one can obtain by using a multi-dimensional approach.

Chairs: Iain Oswald and Anna Warren

Lynne Thomas (Bath)

*Beyond the structure: investigating physical
properties in molecular materials*

Andrew Goodwin (Oxford)

Frameworks, Flexibility and Frustration

Protein Crystallography in Drug Discovery: Binding Sites in the Spotlight

(BSG Session)

The session will cover aspects of protein crystallography in a drug discovery setting, including issues arising during ligand fitting, as well as new structure-guided inhibitor design possibilities opened up with the structure elucidation of G-Protein Coupled Receptor structures.

Chair: Robert Van Montfort

Judit Debreczeni (AstraZeneca, Alderley Park)

*Practical considerations in
ligand substructure validation*

Andy Dore (Heptares Therapeutics)

*Structure Based Drug Design for
the human A2a G-Protein Coupled Receptor*

David Robinson (University of Dundee)

*Structural Biology in Academic Drug Discovery –
Perspectives from the Dundee Drug Discovery Unit*

INTERDISCIPLINARY FORUM

5.15-6.16 pm Forum

Bridging the Gap Between MX and Small Molecule Crystallography

Introduced by Arwen Pearson and Amber Thompson

As small molecules get larger, the challenges they pose increasingly approach those associated with macromolecular crystallography. However, with the divergence of the two fields, we now talk different languages as well as have different scientific backgrounds. This forum is intended to help break-down these barriers through the medium of questions with a panel of experts. Possible questions for discussion include, "What is R_{free} ?"; "How do you judge data quality?"; "How do you prevent solvent loss?" and "What do you do to prevent radiation damage?". The session is short and intended to promote discussion; if successful it could be a prototype for a longer event next year, so suggestions and feedback are greatly encouraged.

Chair: Kirsten E. Christensen

Wednesday 18th April

1.30-3.00 pm Session 4

H-bonding: From Water to Supermolecules I

(Joint PCG and CCG Session)

The session will give an overview of recent theoretical and experimental studies on the condensed phases of water. Specific topics will range from supercooled water and the nucleation of ice at surfaces to stacking disorder in ice.

Chair: Christoph Salzman

Benjamin Murray (Leeds)

*The structure of ice crystallised
from supercooled water*

Angelos Michaelides (UCL)

Ice nucleation at surfaces

Hot Structures and Hot Methods

(BSG Session)

This session consists of talks selected from abstracts reflecting late breaking topics, reports of new structures and updates on new methods.

Chair: Jon Cooper

SAXS

(Joint IG and BSG Session)

The technique of Small Angle X-ray Scattering, in particular biological SAXS, has become increasingly popular in recent years, complementing high resolution structural studies by crystallography, NMR and electron microscopy. Sensitive to length scales in the nanometre range, SAXS can be applied to a wide range of different types of samples including polymers, lipids, nanoparticles, proteins and biomaterials. This session will highlight some recent advances in the field.

Chair: Elizabeth Shotten

Clair Baldock (Manchester)

*Combining SAXS and biophysical techniques to
investigate the nanostructure of extracellular
matrix proteins*

Nick Terrill (Diamond Light Source)

*Small Angle Scattering -
The last resort of the desperate?*

3.30-5.00 pm Session 5

H-bonding: From Water to Supermolecules II

(Joint CCG and PCG Session)

This session focuses on the Crystal Engineering aspects of the hydrogen bond. Intermolecular interactions mediated by hydrogen are frequently structure-defining in organic and metal-organic structures from hydrates, polymorphs and co-crystals right through to highly complex supra-molecular systems. The session will touch on the importance of the hydrogen bond in analysis, design and prediction of small molecule crystal structures.

Chair: Peter Wood

Doris E. Braun (UCL)

*Contrasting organic hydrate structures
generated in silico to in vitro*

Laszlo Fabian (UEA)

Cocrystal design: interactions and properties

Crystallography and Cancer

(BSG Session)

High throughput structural biology approaches can play a pivotal role in the target validation, hit identification, hit-to-lead and lead-optimisation phases of drug discovery. In this session, two pioneers of these approaches will discuss high value and high throughput approaches to unlocking the potential of anti-kinase and anti-chaperone drug targets.

Chair: Jane Endicott

Chris Murray (Astex Therapeutics, Cambridge)

*The application of fragment-based
drug design to drug targets in oncology*

Stefan Knapp (Structural Genomics Consortium,
Oxford)

*Strategies for the structure guided
design of selective kinase inhibitors*

Process Analytical Technology (PAT) for Online Monitoring of Material Quality in Manufacture

(IG Session)

Industrial group session covering the application of PAT for monitoring and controlling the quality of a product during manufacture, as used in the Pharmaceutical and Aggregate/Cement industries.

Chair: Brett Cooper

Ali Saleemi (Loughborough)

*The role of PAT in crystallisation
process monitoring and control*

Thursday 19th April

10.15-11.45 am Session 6

Phase Transitions: Distortion Mode Analysis

(Joint PCG and CCG Session)

The session will connect the fundamentals with the topical materials research and provides the basis for a state-of-the-art diffraction data analysis approach.

Chair: Ivana Evans

Mark Senn (Edinburgh)

The Verwey Structure of Magnetite: Charge Order and Three-Site Distortions

Membrane Protein Crystallography

(BSG Session)

Protein crystallographic analysis of membrane proteins is critical to understanding structure-function relationships and important to understanding disease processes and for the development of new medicines. Only a small subset of independent structures of integral membrane proteins have been reported so far and in this session the technological challenges and recent breakthroughs of research in this important area are explored.

Chair: Jonas Emsley

So Iwata (Imperial College)

Structural studies of integral membrane proteins

Andrew Leslie (Cambridge)

Crystallography of G-protein coupled receptors

Coatings

(IG Session)

Coats of many colours: Probing and understanding surfaces and the coatings interacting with them, is a science that continues to grow as technology becomes more specifically focused on this interesting environment. This session will present lectures from speakers picked across a number of industrial sectors, showing how these surfaces and coatings are important to each and the techniques used to understand the associated challenges.

Chair: Judith Shackleton

Speakers and titles: TBC

12.00-1.30 pm Session 7

Protein Crystallisation: Magic Versus Logic

(BSG Session)

This session will focus on non standard methods for obtaining and optimising macro-molecular crystals using "logic" (i.e. chemical and physico-chemical prior knowledge, crystallisation diagnostic techniques and further means) to counter balance the "magic" ingredient which many regard as essential for producing diffracting crystals.

Chair: Naomi Chayen

Terese Bergfors (Uppsala, Sweden)

Highways, biways and detours: the IspD story

Emmanuel Saridakis (Demokritos, Greece)

Discovering crystallisation conditions using Dual Polarization Interferometry

Phase Transitions II: Transformations in the Solid State

(Joint CCG, IG and PCG Session)

This session is concerned with the transformation of one crystalline form into another as a result of a stimulus such as a change in temperature. The primary tool to monitor such processes is the monitoring of structure before and after transition by diffraction-based techniques. However the field is now increasingly turning to other techniques to probe the kinetics, dynamics and mechanisms of these transitions and complementary techniques such as Calorimetry, Solid State NMR and computational-based calculations are now being employed to further our understanding of these complex processes. The session will draw on all these complimentary approaches in presentations outlining examples from different areas of academia and particularly pharmaceutical relevance.

Chairs: Simon Coles and Cheryl Doherty

Kenneth Harris (Cardiff)

Structural and dynamic aspects of phase transitions in solid inclusion compounds