

The Irish Crystallographic Association
Cumann Criostalagrafaíochta na hEireann

The inaugural meeting of the Irish Crystallographic Association, in collaboration with the British Association for Crystal Growth, was held on Thursday 6th September 2012 in Dublin. The meeting opened with a welcome address in both Irish and English by the Chairman of the ICRA, Patrick McArdle. Here are brief summaries of the presentations:

Keith Lorimer "*The Evolution of Solid Form Screening*" discussed different methods of screening for solid forms, from humble beginnings pioneered by the Kofler husband and wife team, McCrone's first high-throughput experiments, to the vast arrays of methods which are available today, the ICH Q6A & FDA guidelines and the techniques of the future.

Colin Seaton "*Solution Mediated Polymorphic Transformations*" discussed different ways in which polymorphic transformations occur in solution, with reference specifically to sulfathiazole, paracetamol and carbamazepine, as well as computational methods for assisting their understanding.

Brian O'Sullivan "*Recent Advances in in-situ Particle Characterisation*" described improvements in FBRM software and technology which lead to more accurate analytical data and enables better understanding of the nucleation and growth processes, with reference to specific case studies.

Robert Hill "*D8 Crystallography Solutions*" outlined the new generation of single crystal instruments available for high performance crystallography, including the Ga-based METALJET system for significant enhancement of flux.

Gary Morris "*Alternative Processing Technologies and Control for the Selective Crystallization of Desired Polymorphs*" introduced different continuous crystallisation platforms and explained how they can be used to control both morphology and size of crystallising particles, depending on the kinetics of how supersaturation is achieved.

Joseph Lyons "*The rational tailoring of the in meso method - the crystallisation of caa3-type cytochrome oxidase*" described the intricacies involved in membrane protein crystallisation and that it is now possible to tailor a specific monoacylglycerol for the selective crystallisation of membrane proteins, via targeting of the predicted topology of the protein. This was demonstrated with caa3-type cytochrome oxidase.

Sally Price "*Computed Crystal Energy Landscapes as a Complement to Solid State Screening*" outlined the role of crystal structure prediction in crystal polymorphism, and how it has evolved from predicting the most thermodynamically stable structure to understanding the crystal energy landscape. The combination of this with experimental screening techniques is particularly potent in solid form discovery. She highlighted the role of crystal structure prediction in explaining disorder in some systems, as well as highlighting future directions, with particular emphasis on larger molecules, more accurate energies, and increased collaboration between experimentalists and theoreticians.

Finally, a big thank you to our sponsors: British Association of Crystal Growth, Bruker, Mettler-Toledo and Roche for their generous support, without which this meeting would not have been possible.

Simon Lawrence (Secretary) 12th September 2012.