s6.m20.o2 **Nucleation in the Presence of Uncharacterised Impurities.** Richard Sear, *University of Surrey, Department of Physics, Guildford, GU2 7XH United Kingdom. E-mail: r.sear@surrey.ac.uk*

Keywords: Nucleation; Heterogeneous; Impurities

The nucleation of crystals of both small molecules and proteins is almost always heterogeneous, and the nucleus typically forms on a substrate whose nature is unknown. Despite this, historically most theoretical studies of how small molecules and proteins nucleate have looked only at homogeneous nucleation. This is beginning to change and my talk will look at recent attempts to understand heterogeneous nucleation. In particular it will look at attempts to characterise the nucleus in heterogeneous nucleation, for example Auer and Frenkel [Phys. Rev. Lett. v91 015703] have shown that the nucleus can be more like a highly irregular pancake than the sphere of conventional theories of homogeneous nucleation. Also, it will look at how heterogeneous and homogeneous nucleation can lead to different distributions of the sizes of the resulting crystals and on how statistical methods can be used to infer some properties of the impurities using only repeated measurements of the rate of nucleation of the protein or molecule.

s6.m20.o3 **Overcoming Crystallisation Obstacles in the Pharmaceutical Industry.** Neera Borkakoti, *Medivir UK, Peterhouse Technology Park, 100 Fulbourn Road, Cambridge CB1 9PT, UK. E-mail: neera.borkakoti@medivir.com*

Keywords: Crystallisation; Protein; Industry

Technical advances in protein expression, production and purification protocols generally ensures an adequate supply of protein suitable for crystallisation trials. Provided protein crystals suitable for X-ray diffraction have been produced, the developments in the speed and scope of data collection coupled with the progress in computational procedures guarantees an accelerated completion of the structure determination process. This talk will focus on actual examples of processes that have been successfully applied to proteins in order to overcome the traditional bottleneck of protein crystallisation. The role of procedures such as mutagenesis, de-glycosylation and co-crystallisation with ligands will be discussed. Examples will also include structure-based protein modification strategies that have lead to increased crystallisability of the sample.