

Oral Contributions

[MS24-02] Multi-component molecular materials: design, properties, crystallisation, manufacture. Chick C. Wilson.

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The development of new materials using structural chemistry methods is centred around the understanding of hydrogen bonding in molecular systems, including the application of crystal engineering principles that enable us to make predictions about likely molecular associations and ideally to be able to control these. The synthesis domain in which this work is carried out is often the solution-mediated self-assembly environment of a crystallisation experiment, and the transfer of structural chemistry knowledge to crystallisation science including polymorph discovery and control in multi-component environments is a challenge that this work is beginning to address. This includes initial steps towards taking the synthesis of multi-component solid state molecular materials and transferring this into continuous crystallisation flow environments.

In trying to reach the goal of “Directed Assembly” of molecular materials with designed architectures or tuneable properties, controlling the ubiquitous yet challenging hydrogen bond interaction is crucial. The use of relatively simple, robust hydrogen bonded supramolecular synthons that form the building block of multi-component molecular materials can begin to make this achievable. We will discuss attempts to use these not only to control the assembly of molecules and molecular complexes into predicted architectures, but also to design into these systems some degree of structural (and hence functional) tunability.

The multi-component self-assembly environment can also offer different opportunities, for

example in the control of solid form. Recent work on polymorph control and discovery from multi-component self-assembling systems will be discussed. The value of the multi-component crystallisation environment has become increasingly clear, offering simple routes to elusive and previously unknown polymorphs utilising the templating action of benign second molecular components. The selective production of selected forms of single component materials from a multi-component environment will be discussed with reference to a wide range of systems in which this method has recently been successful.

Recognising the high relevance of much of this work in developing and controlling functional multi-component molecular materials, we have recently begun transferring some of our crystal engineering and multi-component self-assembly systems into the flow environment, within the CMAC (Continuous Manufacturing and Crystallisation) project. This targets effective, controlled manufacture of solid form molecular materials with control over crystal form, particle attributes and physical properties in a continuous crystallisation process.

Keywords: multi-component molecular materials; crystal engineering; crystallisation science