Towards an Understanding of Molecular Solids: Challenges, Strategies and Solutions

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The lecture will highlight some contemporary challenges in understanding the properties of molecular solids, and will focus on strategies that may be implemented in the quest to find solutions to these challenges.

The first challenge is how to determine the structures of crystalline solids when single crystals suitable for single-crystal X-ray diffraction (XRD) cannot be prepared. In such cases, structure determination must be tackled using *powder* XRD data. However, the challenges associated with this task are such that, as recently as the early 1990s, no organic crystal structure had ever been determined directly from powder XRD data. Since that time, developments in methodology (particularly the direct-space strategy for structure solution [1]) are such that the crystal structures of organic materials of moderate complexity can now be determined relatively routinely from powder XRD data, as demonstrated by several recent applications [2,3].

In many respects, solid host-guest materials based on one-dimensional tunnel host structures (for example, urea and thiourea inclusion compounds) are ideal model systems for exploring and understanding a wide range of fundamental materials properties. In this regard, our recent research has exploited solid inclusion compounds as model materials for: (i) understanding and controlling crystal growth processes [4,5], and (ii) developing and applying the phenomena of X-ray dichroism and X-ray birefringence [6,7]. The lecture will present an overview of several inter-related aspects of our research on these materials.

The lecture will also highlight recent research on the development of a new solid-state NMR strategy for *in-situ* studies of crystallization processes [8-10].

The lecture is organized in the following sections:

(a) development and application of techniques for structure determination of organic materials from powder XRD data [1-3],
(b) fundamental and applied aspects of solid inclusion compounds [4,5],
(c) the phenomenon of X-ray birefringence [6] and exploitation of this phenomenon as the basis of a new X-ray imaging technique [7] that represents the X-ray analogue of the polarizing optical microscope,
(d) *in-situ* solid-state NMR studies of crystallization processes [8-10].

References

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