Invited Lecture

Cocrystallisation as a Modular Approach to Smart Materials Discovery

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Molecules that change their colour, structure, and electronic properties in response to an external stimulus represent an emerging class of 'smart' material with potential applications in sensing, actuating and cooling technologies. The spin crossover (SCO) phenomenon leads to a redistribution of electrons within the d-orbitals of some transition metal complexes as a result of an external perturbation such as changes in temperature, pressure changes and light irradiation. The transition between high-spin and low-spin states involves a significant change in molecular volume and is often cooperative in crystalline materials, leading to dramatic changes in the optical, mechanical and magnetic properties.

Recent work in our group has shown the significant promise of using cocrystallisation to design new SCO materials with tunable thermally-responsive properties [1,2]. The cocrystals have been studied by variable temperature single-crystal X-ray diffraction and SQUID magnetometry to develop structure–property relationships. The supramolecular architecture of the cocrystals depends on the properties of the coformer. With linear, rigid coformer molecules leading to 1D supramolecular hydrogen-bonded chains, while flexible coformers form 2D sheets and bent coformers yield 3D network structures. The SCO behaviour of the cocrystals can be modified through changing the coformer and thus co-crystallisation presents a rapid, facile and highly modular tool for the discovery of new switchable materials. The wider applicability of this strategy to the design of hybrid multifunctional materials will also be discussed.

1. L.T.Birchall, G.Truccolo, L.Jackson and H.J.Shepherd, Chemical Science, 2022,13, 3176-3186.

2. L.T.Birchall, A.Raja, L.Jackson and H.J.Shepherd, Crystal Growth and Design, 2023, 23, 3, 1768–1774.