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Co-crystallisation and phase-transition: from pharmaceuticals to thermochromics

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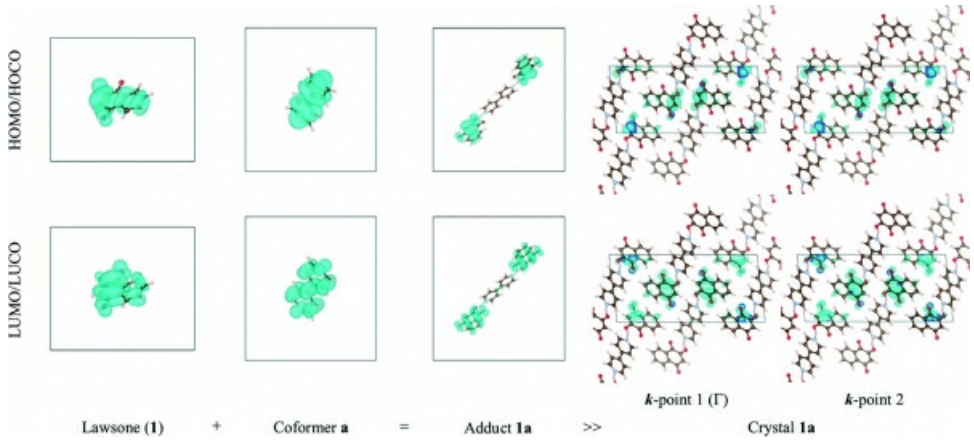
Molecular recognition through hydrogen bonding, halogen bonding, or π-stacking interactions has significant influence on the properties of molecular materials. With thousands of small organic molecules currently known, the possibilities of producing new materials with desired properties using molecular recognition are endless. Together with computational modelling, it is possible now to use co-crystallisation to tailor properties to suit our needs. For example, in pharmaceutics, crystal morphology can greatly influence not only the solubility and bioavailablity of a drug, but also physical properties like processing parameters, with acicular needles being the worst of them all as they tend to clog machinery causing a lot of processing problems; using co-crystallisation makes it possible to modify and improve upon these properties. Another example is that of thermochromic materials. Colour is among the most interesting properties of materials. Apart from being a visual treat, colour gives insight into the electronic structure and interactions within the material. Dyes, pigments, dichoric and thermochromic materials have multiple uses in everyday life, spanning from their use in art to the production of sensors. Co-crystallisation of small molecules can be used to tune the colour of chromophores and to form coloured co-crystals from materials that are otherwise colourless1. When these co-crystals have polymorphs themselves, temperature-induced phase transitions can make the materials thermochromic, and hence a lot more interesting.

Through experimental co-crystal screening, x-ray crystallography, high-resolution spectroscopy and computational studies (e.g. TD-DFT calculations), we have explored a range of materials including diflunisal2 (an anti-inflammatory drug), Lawsone (henna dye used for tattoos and hair colouring) 3, and dinitrobenzoic acids1,. We have managed to identify key features amongst the molecular recognition patterns that alter the properties of these materials.

Figure: Orbital-density plots illustrating the relationship between the frontier orbitals of Lawsone (1), a coformer a, the gas-phase H-bonded adduct 1a, and the corresponding solid form.

1 C. L. Jones (2014). Crystengcomm, 16, 5849–5858.
2 Pallipurath, A. R. (2016). Crystal Growth and Design, 11, 6468-6478
3 A. Pallipurath (2015). CrystEngComm, 17, 7684–7692.



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