Procrystals: Structure and Dynamics

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Functional materials design normally focuses on structurally ordered systems because disorder is often considered detrimental to many functional properties. In a recent study[1] we have sought to challenge this paradigm by showing that particular types of strongly correlated disorder can give rise to useful characteristics that are inaccessible to ordered states. A judicious combination of low-symmetry building unit and high-symmetry topological template leads to aperiodic 'procrystalline' solids that harbour this type of disorder. This talk will introduce key classes of procrystalline states together with their characteristic diffraction behaviour, and establish mappings onto known and target materials. The strongly correlated disorder found in these systems is shown to be associated with specific sets of modulation periodicities distributed throughout the Brillouin zone. Lattice dynamical calculations reveal selective disorder-driven phonon broadening that resembles the poorly understood 'waterfall' effect observed in relaxor ferroelectrics. This property of procrystalline solids suggests a mechanism by which strongly correlated topological disorder might allow independently optimized thermal and electronic transport behaviour, such as required for high-performance thermoelectrics.

1. A. R. Overy, A. B. Cairns, M. J. Cliffe, A. Simonov, M. G. Tucker, A. L. Goodwin, *Nature Comms.*, **7**, (2016), 10445.