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Understanding the Mechanisms Bending in Flexible Crystals

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A crystal is normally thought of as a homogenous solid formed by a periodically repeating, three-dimensional pattern of atoms, ions, or molecules. Indeed, the regular arrangement of molecules, in a single crystal lead to many useful characteristics (in addition to diffraction!) including unique optical and electrical properties, however, molecular crystals are not typically mechanically robust, particularly compared to crystals of network solids like diamond. Upon the application of stress or strain, these crystals generally irreversibly deform, crack or break resulting in the loss of single crystallinity.
We have recently discovered a class of crystalline compounds that display the intriguing property of elastic flexibility – that is they are capable of reversibly bending without deforming, cracking or losing crystallinity. A number of these crystals are flexible enough to be tied into a knot! (See Figure 1). We have developed a unique approach to determine the atomic-scale mechanism that allows the bending to occur which employs mapping changes in crystal structure using micro-focused synchrotron radiation. We have applied this technique to understand the deformation in both elastically1 and plastically2 flexible crystals. Most recently we have used it to show that previous theories regarding the requirement of "interlocked" crystal packing for flexibility is incorrect.

Figure 1: A crystal of [Cu(acac)2] showing elastic flexibility.

A. Worthy, A. Grosjean, M. Pfrunder, Y. Xu, C. Yan, G. Edwards, J. K. Clegg and J. C. McMurtrie, "Atomic Resolution of Structural Changes in Elastic Crystals of Copper(II) acetylacetonate", Nature Chemistry, 2018, 65-69.
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