

## MS31-04 | INSIGHTS FROM HIGH-PRESSURE CRYSTALLOGRAPHY AND X-RAY CHARGE DENSITY ANALYSIS INTO MECHANICAL FLEXIBILITY OF METAL-ORGANIC COMPLEX CRYSTALS

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Crystal engineering studies have provided insights into unusual mechanical phenomena such as crystal bending and shearing - based on anisotropy of intermolecular interactions in crystals. However, as more and more complex and anomalous cases of flexible crystals are being discovered, it demands for quantitative approaches to understand the structural origin and mechanism of such properties. In recent reports, we have shown the utility of novel computational tools and experimental charge density analysis to understand these properties [1,2]. In this presentation, I will discuss the application of high-pressure crystallography using diamond anvil cell (DAC) in understanding the structural changes occurring in flexible molecular crystals upon a homogeneous pressure. We propose that the structural changes at varying pressures can provide valuable information on the intermolecular structural dynamics involved in the mechanism of flexibility in such crystals. The example of an elastically flexible crystal formed by a Copper (II) complex will be discussed, with a focus on the structural changes at molecular and intermolecular level -observed between ambient to high pressures ( $10^{-4}$ -15 GPa). The role of some unusual 'sigma-hole' interactions/bonds in guiding the flexible property of this crystal has been unravelled by synchrotron X-ray charge density model and computational analysis.

[1] M. J. Turner, S. P. Thomas, M. W. Shi, D. Jayatilaka, M. A. Spackman, *Chem. Commun.*, **51**, 3735 (2015).

[2] S. P. Thomas, M. W. Shi, G. A. Koutsantonis, D. Jayatilaka, A. J. Edwards, M. A. Spackman, *Angew. Chem. Int. Ed.* **56**, 8468 (2017).