## MS35-P26 | ORGANIC COCRYSTALS WITH MECHANICALLY INTERLOCKED ARCHITECTURES: UNPRECEDENTEDLY STIFF AND HARD WITH ELASTIC FLEXIBILITY

Dey, Somnath (Institute of Crystallography, RWTH Aachen University, Aachen, GER); Das, Susobhan (Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, IND); Reddy, C. Malla (Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, IND)

Mechanical properties of molecular crystals and their limits of adaptability have attracted tremendous interest among researchers in the recent years. Recent nanoindenation experiments revealed that certain molecular crystals with strong hydrogen bond networks can be as stiff as 44 GPa while theoretical predictions show these values exceeding 100 GPa [1]. However, the very presence of strong H-bonds deters any macroscopic flexibility which is also a key determining factor of candidacy for potential applications. On the other hand, mechanically flexible crystals which comprise overwhelmingly weaker interactions are mostly known to be significantly softer (up to ~18 Gpa).

Here we report an exceptional mechanical stiffness (~78 GPa) and unprecedentedly high hardness (~7 GPa) in an elastically bendable organic cocrystal [caffeine, 4-chloro-3-nitrobenzoic acid and methanol (1:1:1) [2]]. These values are comparable to certain low-density metals and counter intuitive considering the current knowledge. Spatially resolved atomic level studies reveal that (i) mechanically interlocked weak hydrogen bond networks separated by dispersive interactions gives rise to such unprecedented elasticity and hardness; (ii) The bent crystals significantly conserve the overall energy by efficient redistribution of stress; (iii) Perturbations in weak hydrogen bonds are compensated by strengthened π-stacking. Further, we report for the first time a remarkable stiffening (~11%) and hardening (~100%) in the elastically bent crystal. Hence, mechanically interlocked architectures provide an unexplored route to reach new mechanical limits and adaptability in organic crystals.

[1] Angew. Chem. Int. Ed. 2015, 54, 13566 –13570
[2] Angew. Chem. Int. Ed. 2012, 51, 10319 –10323