Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Molecular Mechanics of Elastic and Bendable Caffeine Co-crystals

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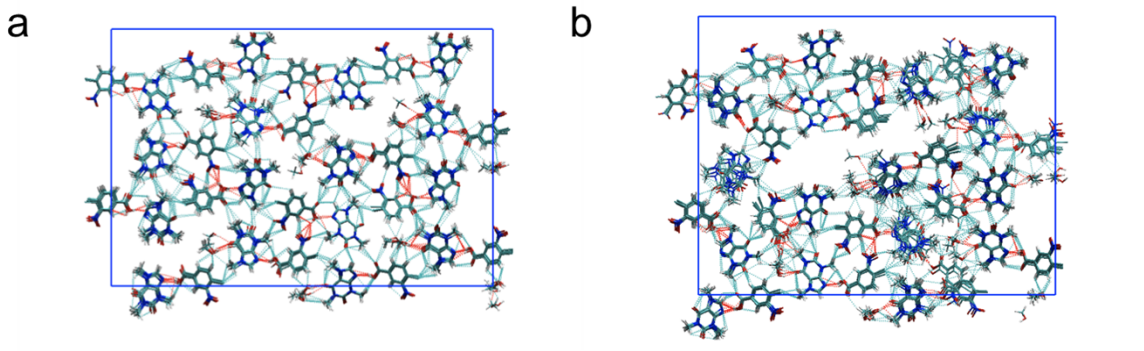

Figure S1 | Breaking mechanisms of hydrogen bond during tensile test. The dashed lines indicate the hydrogen bonds in the cocrystal solvate **1** at **(a)** 10 % tensile strain and **(b)** 20 % tensile strain.

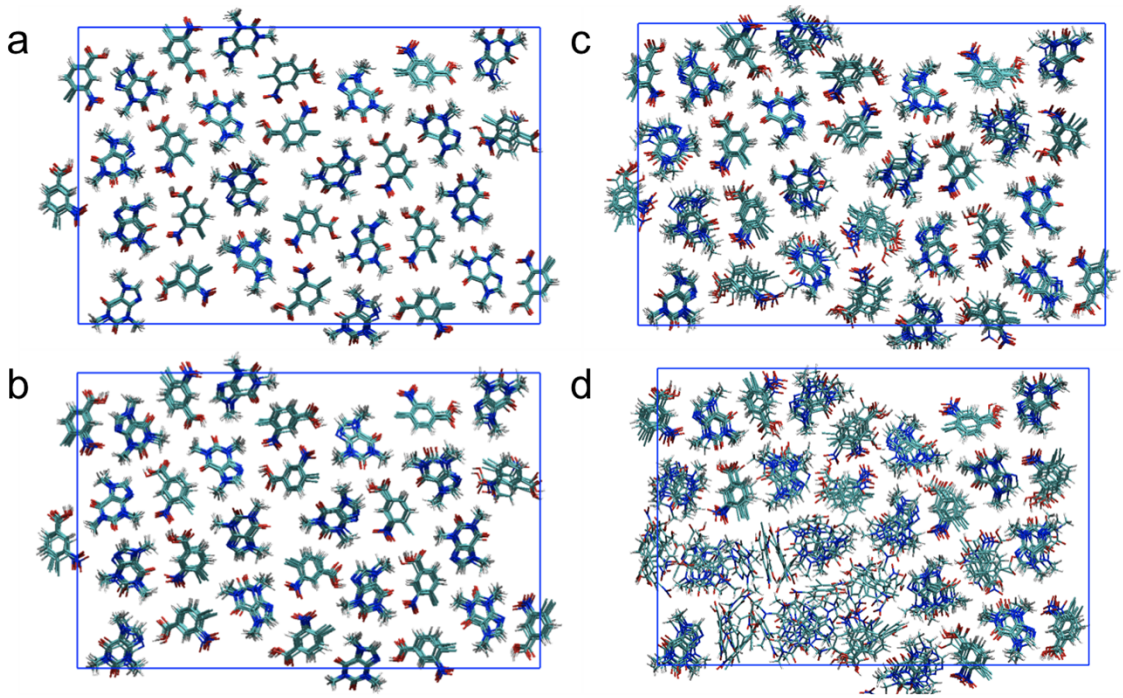

Figure S2 | Snapshots of cocrystal solvate 1 (dry) at different temperatures. View of the crystal packing perpendicular to (001) at temperature of **(a)** 200 K, **(b)** 300 K, **(c)** 400 K, and (**d**) 500K. The blue-boxed region indicates the simulation box.

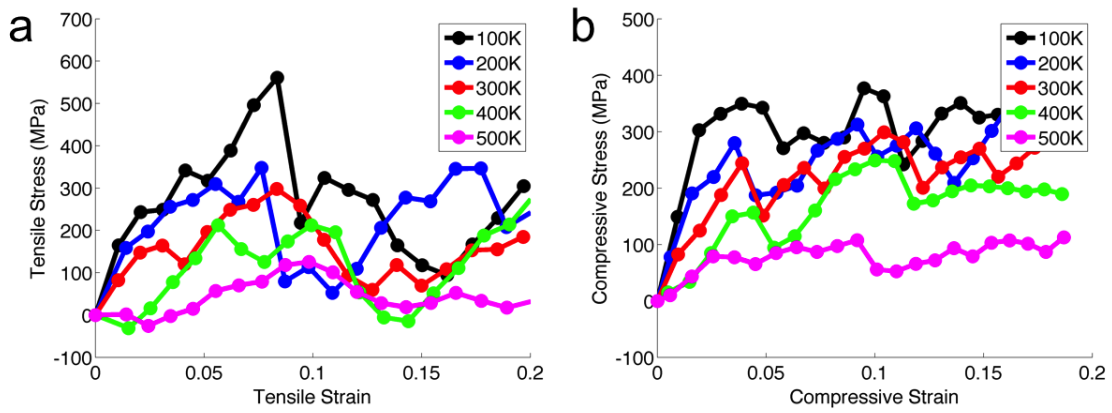

Figure S3 | Stress-to-strain curves of cocrystal solvate 1 (dry). Results of simulated **(a)** tensile test and **(b)** compressive test.

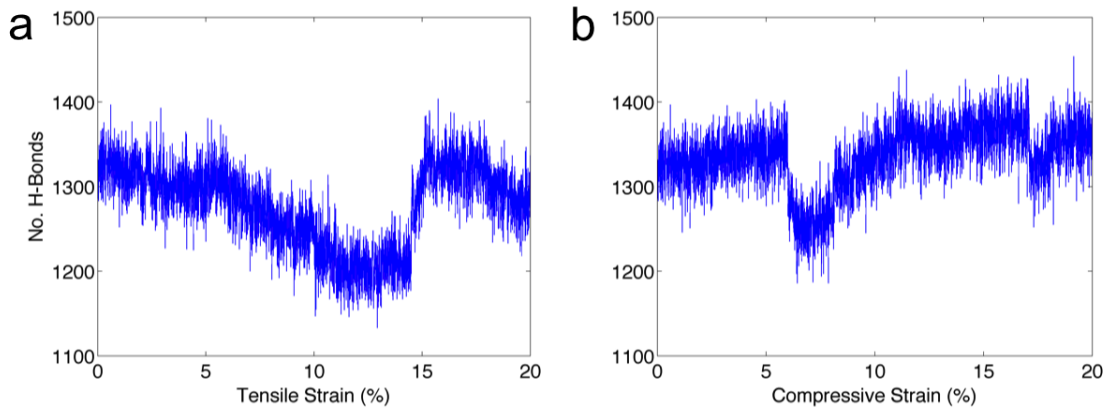

Figure S4 | Number of hydrogen bonds in cocrystal solvate 1 (dry). The number of hydrogen bonds in **1** (dry) during the (**a**) tensile and (**b**) compressive tests. In the calculations, we choose 3.6 Å as the distance cutoff and 80° as the angle cutoff.

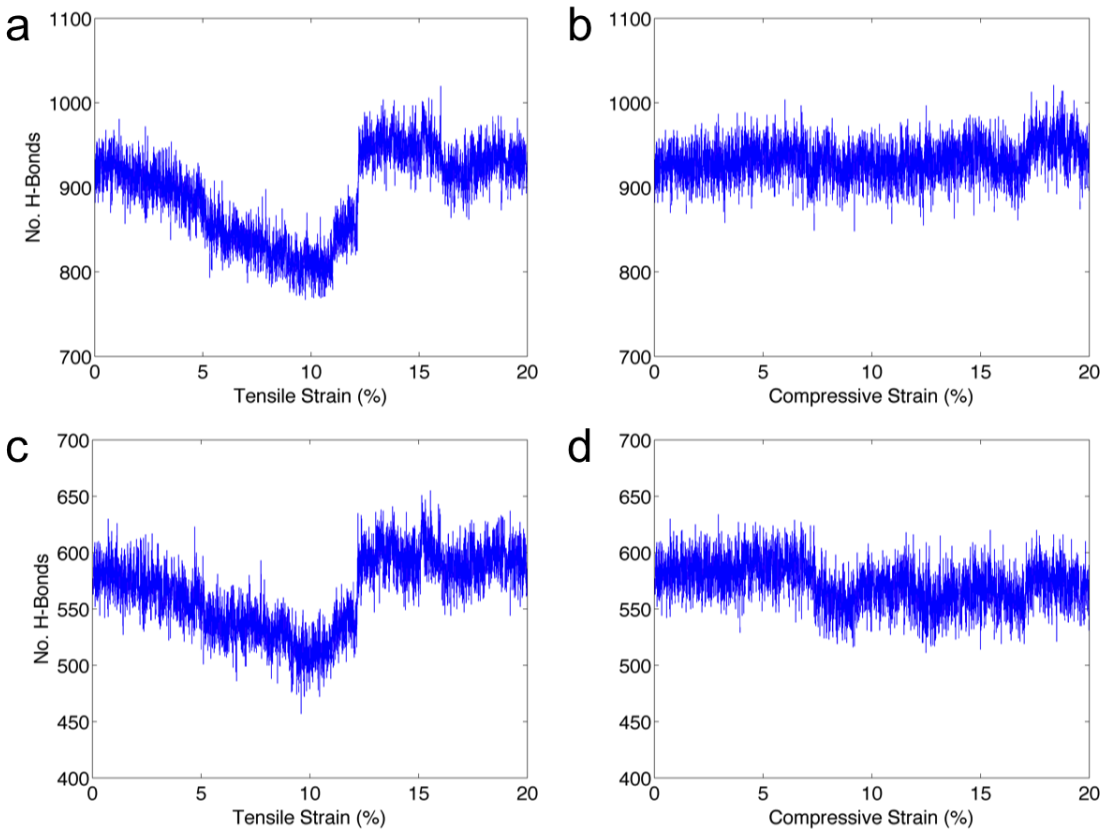

Figure S5 | Number of hydrogen bonds in cocrystal solvate 1 calculated with different angle cutoff. The number of hydrogen bonds in **1** during the (**a**) (**c**) tensile and (**b**) (**d**) compressive tests. In the calculations, we choose 3.6 Å as the distance cutoff. The angle cutoff is **(a) (b)** 70° and **(c) (d)** 60°.