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Shaping crystals using mechanical force: A structural perspective on flexible crystalline coordination polymers of cadmium(II)

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The conventional conception of crystalline materials as static and brittle started to dramatically change with the serendipitous discovery of crystals exhibiting exceptional stimuli-driven mechanical motions.[1] While thermo- and photosalient dynamic effects have been known for more than 50 years, mechanically induced elastic and plastic responses were relatively recently discovered.[2] Attracted by a wide scientific community, this novel, and unexpected crystalline property is firmly shaping a new direction in crystal engineering, a discipline of crystal adaptronics.[3] However, even with the growing number of reported crystals displaying these outstanding mechanically induced phenomena, the structural background endowing the crystalline materials with adaptive properties is still unclear, and systematic in-depth structure-property correlations are a necessity.

Numerous examples of flexible organic crystalline compounds have been reported so far, while only a handful of compliant metal-organic crystals are known. Relatively recently, we showed that crystals of one-dimensional coordination polymers of cadmium(II) halides with pyrazine and pyridine-based ligands are capable of displaying elasticity and plasticity as a response to mechanical stress.[4–7] Interestingly, a group of seven isostructural crystals of cadmium(II) halides with 3-halopyridine ligands displayed a wide spectrum of different mechanically induced responses, from variable plasticity to a diverse elastic bendability, and these were facilitated only by fine-tuning the strength and geometry of intermolecular interactions.[5,6] To further investigate the impact of crystal packing features on bendability, we prepared another class of crystalline cadmium(II) coordination compounds, using slightly modified pyridine ligands by introducing another halogen atom, i.e., 3,5-dihalopyridines. Here we monitor the impact of the additional halogen atom on the pyridine ligand on the crystal morphology, supramolecular architecture, and finally the macroscopic crystal's response. It was found that the observed distinction in the type and the extent of an elastic bendability is controlled by the relative importance of the halogen and hydrogen bonds in the crystal structure, which brings us one step closer to untangling the structural intricacies of the remarkable world of crystal dynamics.

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