Computational Studies of Flexible Cadmium(II) and Copper(II) Coordination Polymers

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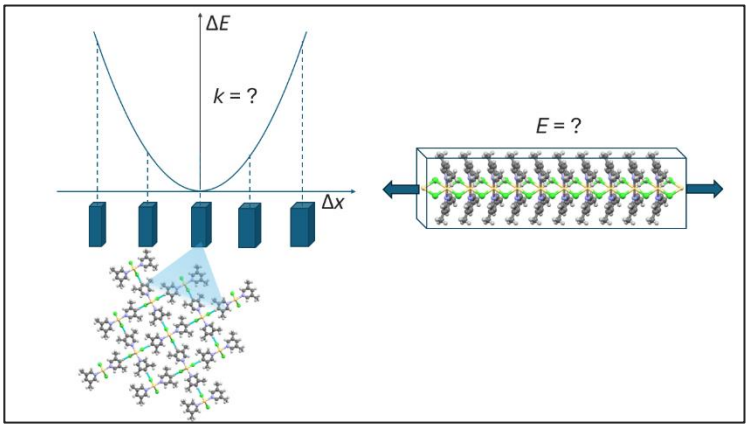
The discovery that crystals can move in response to external light, thermal, or mechanical stimuli has changed the previously held belief that crystals are static systems [1]. When subjected to external mechanical forces, crystals typically bend either elastically or plastically. While numerous organic crystals that dynamically respond to external stimuli have been documented, the number of metal-organic crystal systems with such properties remains limited [2]. Research has shown that one-dimensional coordination polymers are excellent candidates for studying the relationship between mechanical flexibility and structural characteristics [3]. Additionally, it has been established that the explanation for the type of mechanical bending lies in the intermolecular interactions between the building blocks in crystal packing [4]. To gain a deeper understanding of these fascinating crystalline behaviors, we have chosen to study crystals of coordination polymers of cadmium(II) and copper(II) halides with 3,5-dimethylpiridine (**3,5-dmp**): $[CdCl_2(\mathbf{3,5\text{-}dmp})_2]_n$ (**1**), $[CdBr_2(\mathbf{3,5\text{-}dmp})_2]_n$ (**2**), $[CuCl_2(\mathbf{3,5\text{-}dmp})_2]_n$ (**3**), $[CuBr_2(\mathbf{3,5\text{-}dmp})_2]_n$ (**4**). Using computational DFT methods, the deformation of the unit cells along the crystallographic axes was simulated. Comparison of the fitted potential energy curves enabled us to better understand the effect of intermolecular interactions on mechanically induced flexibility. Additionally, Young's moduli of mentioned compounds were calculated and compared with experimental data.



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