

GDR SIGMA-HOLE



16th to 17th June 2025, Universite Paris-Saclay

Halogen bonds in the functioning of mechanoflexible crystals

Marijana Đaković¹ ¹ Department of Chemistry, Faculty of Science, University of Zagreb, Zagreb, Croatia ² Affiliation 2 (Calibri 10) <u>e-mail mdjakovic@chem.pmf.hr</u>

The conventional view of crystals as static, inflexible structures has been fundamentally transformed in recent decades, thanks to substantial evidence highlighting their dynamic capabilities. Research has conclusively demonstrated that crystals are able to exhibit a remarkable array of behaviours—jumping, exploding, flexing, peeling, and even crawling—reacting to various external stimuli such as heat, electric or magnetic fields, mechanical forces, and light.^[1] When we delve into the impact of mechanical force, it becomes evident that crystals can display elastic flexing by returning to their original shape upon removal of the force, or undergo plastic deformation that leads to a permanent change in the crystal shape. Furthermore, certain crystals seamlessly combine these behaviours, showcasing their elastoplastic properties. This evolving understanding highlights the intricate and responsive nature of crystals, revealing their exceptional ability to adapt to their environment.

In this work, we concentrate on the flexible properties of crystals as they respond to applied mechanical forces, aiming to understand the role of intermolecular interactions in the behaviour of these fascinating materials. Our primary focus is on crystalline coordination polymers, which have emerged as a promising class of crystalline materials for investigating the structural foundations and principles that contribute to targeted flexibility.^[2–6] Furthermore, these materials have allowed us to highlight supramolecular interactions as critical factors influencing a range of distinct mechanical responses. This contribution will specifically explore the role of halogen bonds in these captivating crystal behaviours.

References:

[1] Awad, W. M.; Davies, D. W.; Kitagawa, D.; Halabi, J. M.; Al-Handawi, M. B.; Tahir, I.; Tong, F.; Campillo-Alvarado, G.;

Shtukenberg, A. G.; Alkhidir, T.; Hagiwara, Y.; Almehairbi, M.; Lan, L.; Hasebe, S.; Karothu, D. P.; Mohamed, S.; Koshima, H.; Kobatake, S.; Diao, Y.; Chandrasekar, R.; Zhang, H; Sun, C. C.; Bardeen, C.; Al-Kaysi, R. O.; Kahr, B.; Naumov, P. *Chem. Soc. Rev.* **2023**, 52, 3098.

^[2] Đaković, M.; Borovina, M.; Pisačić, M.; Äakeroy, C. B.; Kukovec, B.-M.; Soldin, Ž.; Kodrin, I. Angew. Chem. Int. Ed. 57 (2018) 14801.

^[3] Pisačić, M.; Kodrin, I.; Trninić, A.; Đaković, M. Chem. Mater. 2022, 34, 2439.

^[4] Pisačić, M.; Biljan, I.; Kodrin, I.; Popov, N.; Soldin, Ž.; Đaković, M. Chem. Mater., 2021, 33, 3660.

^[5] Pisačić, M.; Kodrin, I.; Biljan, I.; Đaković, M. CrystEngComm, 2021, 23, 7072.

^[6] Mišura, O.; Pisačić, M.; Borovina, M.; Đaković, M. Cryst. Growth Des. 2023, 23, 1318.