Oral presentation

On-demand polymorphism *via* lattice dynamics engineering

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The design and synthesis of molecular crystals is rapidly becoming one of the most active fields in solid-state chemistry, given its enormous economic impact on many fields, such as the production of pharmaceuticals, pigments, fertilizers, pesticides, energy-related materials, magnetic materials, organic semiconductors, porous systems. In this context, controlling polymorphism, namely the occurrence of multiple crystal forms for a given set of starting molecular building blocks, is still an open technological challenge that needs to be addressed for the reliable manufacturing of crystalline functional materials.

Here, we explored the rich dynamic landscape of organic crystals [1, 2] uncovering the link between lattice dynamics and polymorphism to devise a series of 13 organic crystals possessing molecular fragments undergoing Brownian motion driving cooperative shapeshifting phase transitions, Figure 1 [3, 4] These results introduce for the first time a reliable strategy to design polymorphic molecular crystalline materials endowed with specific molecular-scale and macroscopic dynamics.

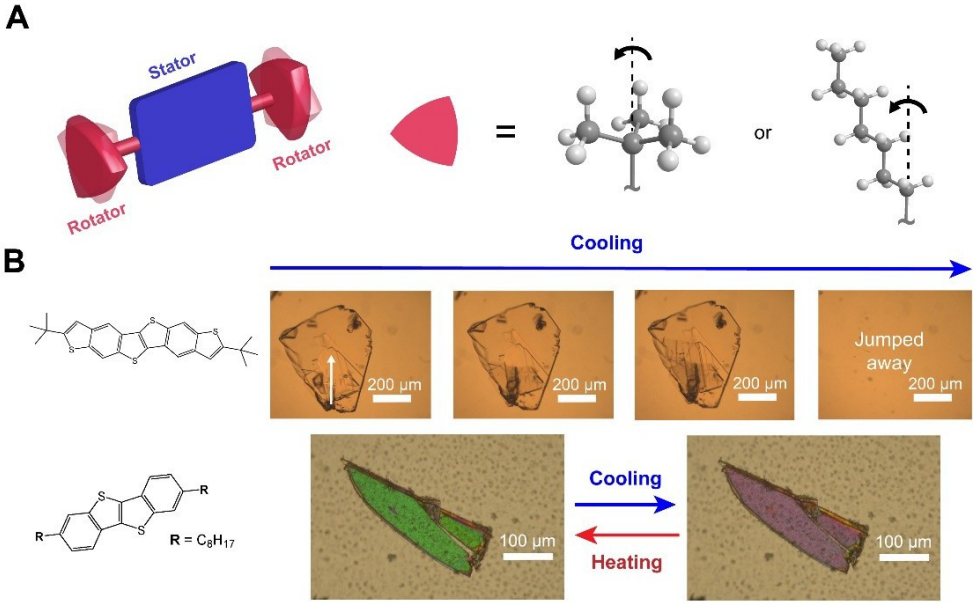

Figure 1. (A) Scheme of the molecular strategy employed. (B) 2 examples of molecular crystals undergoing temperature-induced cooperative phase transitions.

[1] Catalano, L.; Naumov, P. (2018) *CrystEngComm*, **20**, 5872.

[2] Naumov, P.; Karothu, D.P.; Ahmed, E.; Catalano, L.; Commins, P.; Mahmoud Halabi, J.; Al-Handawi, M.B.; Li, L. (2020) *J. Am. Chem. Soc.* **142**, 13256.

[3] Asher, M.; Bardini, M.; Catalano, L.; Jouclas, R.; Schweicher, G.; Liu, J.; Korobko, R.; Cohen, A.; Geerts, Y.; Beljonne, D.; Yaffe, O. (2023) *J. Phys. Chem. Lett.*, **14**, 1570.

[4] Manuscript in preparation.