

MS31. Tailored physical properties in molecular crystals

Chairs: Sebastien Pillet, Pilar Gomez-Sal

MS31-O1 Quantification, systematics and modeling of mechanical effects in molecular crystals

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Elastic materials that are capable of stimuli-responsive mechanical reconfiguration are indispensable for fabrication of mechanically tunable elements for actuation and energy harvesting, including flexible electronics, artificial muscles, and microfluidic elements. The advanced materials that will qualify for these applications in the future must fulfill an extended list of requirements including reversibility, rapid and controllable mechanical response that is proportional to the applied stimulus, and extended lifetime without fatigue.

Elastic properties are counter-intuitive for single crystals of molecular materials which are normally perceived as stiff and brittle entities. The growing realization that bending, curling, twisting, jumping and other mechanical effects of single crystals are surprisingly common has inspired researchers to control crystal motility for actuation. However, new mechanically responsive crystals are reported at a greater rate than their quantitative photophysical characterization; a quantitative identification of measurable parameters and molecular-scale factors that determine the mechanical response has yet to be established. We have recently developed an overarching model for the mechanical effects in crystals that aids our understanding of the macroscopic measurables that could be used for quantification and comparison of the performance of different mechanical effects. The results provide a basis for direct correlations with the molecular and crystal structure.

References:

- [1] M. Panda, S. Ghosh, N. Yasuda, T. Moriwaki, G. Dev Mukherjee, C. M. Reddy, P. Naumov, *Nature Chem.*, 2015, 7, 65.
- [2] M. Panda, T. Runčevski, S. C. Sahoo, A. Belik, N. K. Nath, R. Dinnebier, P. Naumov, *Nature Commun.*, 2014, 5, 4811.
- [3] N. K. Nath, M. Panda, S. Sahoo, P. Naumov, *CrystEngComm*, 2014, 16, 1850.
- [4] R. Medishetty, A. Husain, Z. Bai, T. Runčevski, R. E. Dinnebier, P. Naumov, J. J. Vittal, *Angew. Chem., Int. Ed.*, 2014, 53, 5907.

[5] N. K. Nath, L. Pejov, S. Nichols, C. Hu, N. Saleh, B. Kahr, P. Naumov, *J. Am. Chem. Soc.*, 2014, 136, 2757.

[6] S. C. Sahoo, M. K. Panda, N. K. Nath, P. Naumov, *J. Am. Chem. Soc.*, 2013, 135, 12241.

[7] P. Naumov, S. C. Sahoo, B. A. Zakharov, E. V. Boldyreva, *Angew. Chem., Int. Ed.*, 2013, 52, 9990.

[8] S. C. Sahoo, S. B. Sinha, M. S. R. N. Kiran, U. Ramamurty, A. Dericioglu, C. M. Reddy, P. Naumov, *J. Am. Chem. Soc.*, 2013, 135, 13843.

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