Keynote–14 –250823

Crystal Adaptronics: Intersectional and Collective Properties and Effects of Dynamic Molecular Crystals

P. Naumov

Smart Materials Lab, New York University Abu Dhabi, United Arab Emirates; Center for Smart Engineering Materials, New York University Abu Dhabi, United Arab Emirates; Molecular Design Institute, New York University, NY, USA

pance.naumov@nyu.edu

Keywords: molecular crystals, dynamic properties, smart materials

The anticipated shift in focal point of interest of solid- state chemists, crystal engineers and crystallographers from structure to properties to function of organic solids parallels the need to apply our accumulated understanding of the intricacies of crystal structure to explaining the related properties, with the ultimate goal of harnessing that knowledge in applications that require soft, light-weight, and/or biocompatible organic solids. In these developments, the adaptive molecular single crystals warrant a particular attention as a new class of materials for light, flexible, and environmentally benign devices, primarily memories, capacitors, sensors, and actuators. Some of the outstanding requirements for application of these dynamic materials as high-efficiency energy storage devices are strongly induced polarization, high switching field, and narrow hysteresis in reversible dynamic processes. However, having been studied almost exclusively by crystallographers, molecular crystals still lack the appropriate investigations that reliably evaluate their reproducibility, scalability, and actuating performance, and some important drawbacks have diverted the interest of engineers from these materials. United under the umbrella term *crystal adaptronics*, the recent research efforts aim to realistically assess the appositeness of dynamic crystals for applications that require fast, reversible and continuous operation over prolonged periods of time [1-13]. With the aim to highlight the most recent developments in the research of adaptive molecular crystals, this lecture discusses their assets and pitfalls. Using machine learning for the first time, we identify inherent features and structure-function relationships that fundamentally impact the mechanical response of dynamic molecular crystals. Our approach factors in different crystal properties in tandem and deciphers their intersectional and combined effects on the dynamic performance. It also provides some hints on the likely future developments that capitalize on the untapped, sequestered potential for applications of this distinct materials class.

[1] Mahmoud Halabi, J., Al-Handawi, M. B., Ceballos, R., Naumov, P. (2023) *J. Am. Chem. Soc*. doi: 10.1021/jacs.3c02184
[2] Awad, W. M., Davies, D. W., Kitagawa, D., Mahmoud Halabi, J., Al-Handawi, M. B., Tahir, I., Tong, F., Campillo-Alvarado, G., Shtukenberg, A. G., Alkhidir, T., Hagiwara, Y., Almehairbi, M., Lan, L., Hasebe, S., Prasad Karothu, D., 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. (2023) *Chem. Soc. Rev.* **52**, 3098.
[3] Karothu, D. P., Mahmoud Halabi, J., Ahmed, E., Ferreira, R., Spackman, P. R., Spackman, M. A., Naumov, P. (2022) *Angew. Chem. Int. Ed.* **61**, e202113988.
[4] Spackman, P. R., Grosjean, A., Thomas, S. P., Karothu, D. P., Naumov, P., Spackman, M. A. (2022) *Angew. Chem. Int. Ed.* **134**, e202110716.
[5] Mahmoud Halabi, J., Ahmed, E., Sofela, S., Naumov, P. (2021) *Proc. Nat. Acad. Sci. USA* **118**, e2020604118.
[6] 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.
[7] Commins, P., Al-Handawi, M. B., Karothu, D. P., Raj, G., Naumov, P. (2020) *Chem. Sci*. **11**, 2606.
[8] Karothu, D. P., Mahmoud Halabi, J., Li, L., Colin-Molina, A., Rodríguez-Molina, B., Naumov, P. (2020) *Adv. Mater.* **32**, 1906216.
[9] Ahmed, E., Karothu, D. P., Warren, M., Naumov, P. (2019) *Nat. Commun.* **10**, 3723.
[10] Li, L., Commins, P., Al-Handawi, M. B., Karothu, D. P., Mahmoud Halabi, J., Schramm, S., Weston, J., Rezgui, R., Naumov, P. (2019) *Chem. Sci.* **10**, 7327.
[11] Ahmed, E., Karothu, D. P., Naumov, P. (2018) *Angew. Chem. Int. Ed.* **57**, 8837.
[12] Commins, P., Tilahun D. I., Karothu, D. P., Panda, M. K., Naumov, P. (2016) *Chem. Commun.* **52**, 13941.
[13] Naumov, P., Chizhik, S., Panda, M. K., Nath, N. K., Boldyreva, E. (2015) *Chem. Rev.* **115**, 12440.