Poster

Effect of X-ray radiation on structure and properties of molecular crystals: from damage to a fine tuning

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The interaction of intense synchrotron radiation with molecular crystals frequently modifies the crystal structure by breaking bonds, producing fragments and hence inducing disorder. Moreover, X-ray radiation may strongly affect physical properties such as electronic configurations [1], colour, compressibility, thermal expansion [2], and stability of certain structural forms [3, 4]. Understanding and controlling these radiation effects might offer new possibilities to deliberately tune physical properties of small molecule materials.

Spontaneous lattice deformations are commonly associated with a structural process such as phase transition, spin crossover phenomena, intercalation of battery materials, gas uptake and release - to mention a few. Radiation damage also affects the unit cell dimensions [2] and corresponding strain might promote or supress the structural processes intrinsically coupled to the lattice strain.

A 2nd rank tensor of radiation-induced lattice strain has been recently proposed to characterise the structural susceptibility to radiation [5]. The underlaying material property comprises both the elastic anisotropy of the host lattice and the anisotropy of defect-related chemical potential. Using spin crossover in a molecular crystal as example [6], we show how radiation damage serves as tuning tool for structural process that are sensitive to the lattice strains.

[1] H. Ishibashi, T. Y. Koo, Y. S. Hor, A. Borissov, P. G. Radaelli, Y. Horibe, S-W. Cheong, and V. Kiryukhin, Phys. Rev. B **66**, 144424 (2002)

[2] Coates, C. S., Murray, C. A., Bostrom, H. L. B., Reynolds, E. M. & Goodwin, A. L. (2021). Mater. Horiz. 8, 1446–145

[3] Grzechnik, A., Petrıcek, V., Chernyshov, D., McMonagle, C., Geise, T., Shahed, H. & Friese, K. (2023). Acta Cryst. B, 79(2), 104–113

[4] Bogdanov, N. E., Zakharov, B. A., Chernyshov, D., Pattison, P. & Boldyreva, E. V. (2021). Acta Crysta. B 77(3), 365–370

[5] McMonagle, C. J., Fuller, C. A., Hupf, E., Malaspina, L. A., Grabowsky, S. & Chernyshov, D. (2024). *Acta Cryst.* B 80, 13–18

[6] Chernyshov, D., Dyadkin, V. & Törnroos, K. W. (2022). Acta Crystallographica Section B 78(3 Part 1), 392–396