Oral presentation

Exploring an X-ray Induced Transition in a Rare-Earth Metal–Organic Framework: Tb-CU-10

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Metal–organic frameworks (MOFs) are porous crystalline materials that consist of metal ions or clusters linked by organic ligands. MOFs have been synthesised using several elements including rare-earth (RE) elements such as scandium, yttrium and terbium. RE- MOFs are attractive not only due to their permanent porosity, tuneable pore size/shape and accessible Lewis acidic sites but also due to their distinct optical properties [1]. In our attempts to explore the photoinduced structural dynamics of RE-MOFs using pink Laue time-resolved photocrystallography, we found out that Tb-CU-10 [2] (CU = Concordia University) undergoes to an unknown transition under exposure to X-rays. The transition consists of a colour change from yellow to red and a quenching of its luminescence upon photoexcitation at 390 nm. Further investigation using monochromatic single crystal X-ray diffraction (SCXRD) pinpointed specific energies (15, 25 and 30 KeV) for the transition to take place. Intriguingly, this transition occurs outside of the absorption edge of Tb (~8 KeV). The experiments also reveal that the new X-ray induced phase is metastable and dependent of the temperature. While the new phase can live for several hours at 100 K (Figure 1), it only lives few seconds at 250 K. Despite the vast terrain for exploration, we present our first findings and hypothesis concerning the origins of the phenomenon.

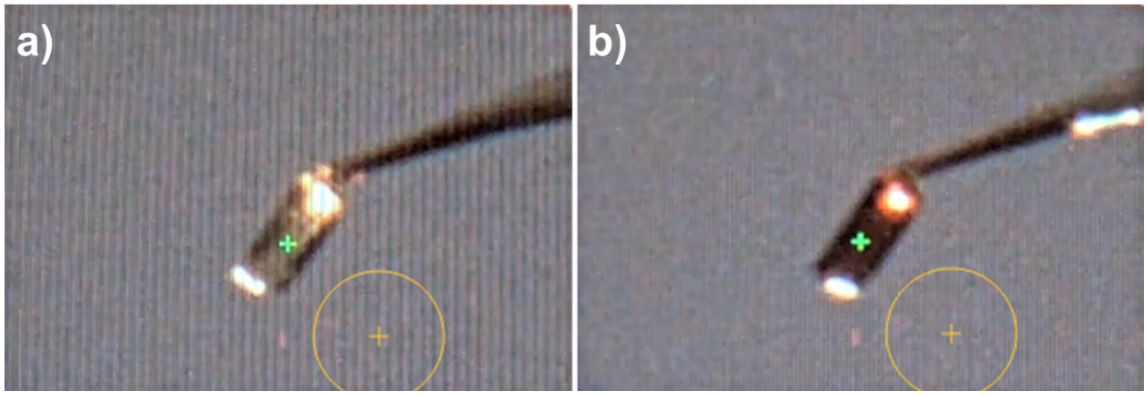

Figure 1. Tb-CU-10 crystal a) before and b) after exposure to X-rays (15 KeV) at 100K.

[1] Saraci, F., Quezada-Novoa, V., Donnarumma, P. R. & Howarth, A. J. (2020) *Chem. Soc. Rev.* **49**, 7949–7977

[2] Quezada-Novoa, V., Titi, H. M., Sarjeant, A. A. & Howarth, A. J. (2021) *Chem. Mater.* **33**, 4163–4169

This research used resources of the Advanced Photon Source, a US Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357. Use of BioCARS was also supported by the National Institute of General Medical Sciences of the National Institutes of Health under grant number P41 GM118217. Time-resolved set-up at Sector 14 was funded in part through a collaboration with Philip Anfinrud (NIH/NIDDK). The content is solely the responsibility of the authors and does not necessarily represent the official views of the National Institutes of Health. Portions of this research were carried out at the light source PETRA-III at DESY, a member of the Helmholtz Association (HGF). We would like to thank P24 staff for assistance in using beamline P24. The current work has been funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – 217133147/SFB 1073, projects B06, C02. HG-recruitment, HG- Innovation "ECRAPS", HG-Innovation DSF/DASHH and CMWS.