Dynamic X-ray diffraction for the design of functional photoswitches

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Switchable crystalline materials are of great and continuing interest for a wide range of smart technologies, with applications including ultrafast electronics, data storage, sensors, molecular machines, solid-state cooling, and energy harvesting.[1-5] In-situ crystallographic studies are a crucial tool for understanding the key structure-property relationships that govern switching in these systems and there are now a wide range of in-situ methods developed for use both in the home X-ray lab and at National Facilities. Our group is particularly interested in studying photoswitchable crystals, and is involved in designing a range of new photocrystallographic equipment and methodologies. These include the development of time-resolved single-crystal X-ray diffraction studies, including stroboscopic pump-probe measurements using synchrotron radiation[6] and a bespoke laboratory set-up, as well as novel serial synchrotron photocrystallography methods.

This presentation will discuss the breadth of this development work, illustrating with example studies of switchable crystals capable of high levels of single-crystal-to-single-crystal conversion. These include photoactive solid-state linkage isomer complexes and, in more recent work, electrically-switchable materials for pyroelectric applications.[7, 8] The latter materials have been studied at Diamond Light Source, using the new in-situ electric field cell available on Beamline I19,[9] and show promise as a new class of rationally-designed systems capable of both photo- and pyroelectric switching in the single-crystal.

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