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Ultrafast Pair Distribution Function Measurements of Local Structural Dynamics in CuIr_2S_4

The Pair Distribution Function (PDF) method interprets Total Scattering data in real space [1]. This distinguishes local structure from the long-range average using information contained within diffuse scattering. xFEL facilities provide the potential to apply this tool to pump-probe experiments and local structural dynamics on the native (sub-)picosecond response timescale of a material.

We show an application of ultra-fast pump-probe PDF (uf-PDF) to CuIr_2S_4 . Below 226 K, the regular Ir sublattice of this material forms Ir-Ir dimers with long range order [2][3]. Using uf-PDF, a decrease in dimerisation is seen within 1 ps of optical pumping. The local (< 1 unit cell) and long-range structures display distinct dynamical behaviours with the long-range structure continuing to evolve over 10s of ps as the pumped phase orders over increasing distances.

[1] Egami & Billinge, ISBN: 9780080971339

[2] Bozin et. al., DOI: 10.1038/s41467-019-11372-w

[3] Radaelli et. al., DOI: 10.1038/41

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