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Simulating Real Space Changes in Cu(DCNQI)₂ Using Ultrafast Electron Diffraction Data

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Well-established X-ray crystallography techniques allow for full steady-state structural analysis of unknown samples. Ultrafast Electron Diffraction (UED) has the added advantage of being able to look at structural properties of samples upon photoexcitation as a function of time, with sub-picosecond temporal resolution. While combining sensitivity to molecular structure with ultrafast timescales is a powerful tool to study ultrafast structural properties of crystals, UED is unable to determine structures like a 'real' crystallographer can. The lack of many observable diffraction orders and the absence of phase information in the electron diffraction patterns, somewhat limits the structural properties extractable from experimental data. This poster discusses how, by utilising prior structural knowledge obtained by steady-state crystallography, it is still possible to obtain real space information about electron diffraction patterns obtained with UED.

Our UED study is done on the organic radical ion salt Copper Methyl,Bromide-Dicyanochino-Diimine, abbreviated as Cu(Me,Br-DCNQI)₂. When this one dimensionally conducting crystal is cooled, it undergoes a structural phase transition at 155 K, whereby three crystal layers trimerise and the material becomes an insulator. This transition can also be photo-induced, making the sample a suitable candidate for UED studies.

During cooling of the sample, the tetrahedral geometry of the crystal distorts, causing the material to undergo the transition. The distortion parameters (i.e. how does the tetrahedral change shape upon cooling) are determined in previous X-ray studies. Using this knowledge, we attempt to interpret observed intensity shifts in our UED data by computationally simulating electron diffraction patterns from known structure files. The ultimate goal of combining electron diffraction simulation studies with experimental UED data is to fully reconstruct real-space changes in Cu(Me,Br-DCNQI)₂ as it undergoes the photo-induced phase transition, as a function of time, thereby creating a 'molecular movie'.

Apply to be
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Yes

Level for award
 (Hons, MSc,
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PhD

Main supervisor (name and email)
and his / her institution

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Would you like to
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Yes

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