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Investigating the insulator-metal phase transition in organic Cu(DCNQI)₂ salts by Ultrafast Electron Diffraction

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Ultrafast electron diffraction (UED) is used to study photo-induced structural phase transitions and dynamics in crystalline materials, with high temporal (sub-ps) and spatial (sub-Angstrom) resolution. Such research can offer insight into the interactions between the different vibrational and electronic degrees of freedom of the material.

The radical anion Cu-dicyanochino-diimine [Cu(DCNQI)₂] molecular crystals have metallic one-dimensional conductivities at room temperature. Particular chemical derivatives of Cu(DCNQI)₂ undergo a periodic lattice distortion (PLD) upon cooling, where the crystal layers along the conducting axis group into sets of three. The PLD is associated with the formation of a charge density wave (CDW) and a dramatic metal-to-insulator phase transition within 1 K, in some cases with a drop in conductivity of eight orders of magnitude. The insulator-to-metal phase transition can be optically driven, making Cu(DCNQI)₂ salts perfect candidates for UED experiments.

We study 50 nm thick, monocrystalline slices of Cu(Me,Br-DCNQI)₂, bulk needles of which undergo a metal-to-insulator phase transition at 155 K. Satellite peaks first appear upon cooling at approximately 165 K, evidence of the PLD and that the crystal has entered its insulating phase. Analysis of the satellite peak intensity and full width half maximum with respect to temperature suggest a gradual crystal layer displacement occurring in crystal domains, which grow together at lower temperatures. Once the sample is in its insulating phase, the insulator-to-metal phase transition can be optically induced. UED experiments show that upon pumping, the satellite peaks are fully suppressed within 2 ps and recover within 40 ps. That is, the PLD is fully reverted and the crystal enters its conducting phase within 2 ps, and recovers to the insulating state within 40 ps. This is accompanied by an ultrafast intensity redistribution of the Bragg peaks on a similar time scale, indicating structural changes in the organic molecules. Interpretation of the Bragg intensity changes will ultimately lead to a real-space 'molecular movie' of the dynamics within the crystal.

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Main supervisor (name and email)
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Heinrich Schwoerer, Stellenbosch University

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Primary author: Ms PAYNE, Nancy (Stellenbosch University)

Co-authors: Mr SMIT, Bart (MSc Student); Prof. SCHWOERER, Heinrich (Stellenbosch University)

Presenters: Mr SMIT, Bart (MSc Student); Ms PAYNE, Nancy (Stellenbosch University)

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