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Ultrafast studies of lattice changes in organic Cu(DCNQI)₂ salts

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Ultrafast electron diffraction (UED) is used to study photo-induced structural phase transitions and dynamics in crystalline materials. UED uses the pump-probe technique: the sample is optically excited by a laser pulse and then its structure is probed by an electron pulse, effectively acquiring a sub-ps snapshot of the crystal structure in time. By changing the time delay between pump and probe, a 'molecular movie' of the induced dynamics can be built up. Such experiments require free-standing and ultrathin (<70 nm) samples.

An interesting candidate for study by UED is the radical anion salt Cu-dicyanochino-diimine [Cu(DCNQI)₂], molecular crystals which exhibit extremely high, one-dimensional conductivities. Even more interesting, particular chemical derivatives of Cu(DCNQI)₂ undergo an abrupt metal-to-insulator (M-I) phase transition upon cooling, with a drop in conductivity of up to eight orders of magnitude within a single Kelvin. The M-I transition is associated with a periodic lattice distortion (PLD) and the grouping of crystal layers along the conducting axis into sets of three. This structural change can be observed in electron diffraction patterns via the appearance of satellite peaks once the crystal has entered its insulating state. The chemical composition of the Cu(DCNQI)₂ salts is highly tuneable, with flexible choice of rest groups, metal ion and extent of deuteration. Changes in composition allow the conductivity and phase transition properties (i.e., the transition temperature) to be systematically and controllably tailored.

The insulator-to-metal phase transition can be optically driven by a laser pulse, thus the induced molecular dynamics can be studied with UED. We study Cu(Me,Br-DCNQI)₂, bulk needles of which have a transition temperature of 155 K. Analysis of the structural changes upon cooling (i.e., steady-state diffraction patterns) and upon photo-excitation (i.e., time-resolved diffraction patterns) will ultimately lead to a full molecular movie of Cu(Me,Br-DCNQI)₂ as it is pumped from its insulating to metallic phase.

Apply to be
 considered for a student
   award (Yes / No)?

Yes

Level for award
 (Hons, MSc,
   PhD, N/A)?

MSc

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

Heinrich Schwoerer, Stellenbosch University

Would you like to
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 Proceedings (Yes / No)?

No

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