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Commensurate charge density wave formation in a novel organic molecular conductor (DCNQI) and tantalum diselenide (4Hb-TaSe2) crystals

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Abstract content
   (Max 300 words)
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Electron diffraction simulation models are used to investigate structural dynamics in a novel organic molecular conductor (Cu [2, 5-CD3-DCNQI]2) crystals and tantalum diselenide (4Hb-TaSe2 cystals). DCNQI crystals undergo photo-induced Peierl's phase transition from a conducting (room temperature) to an insulating phase (Tc = 73 K). A phenomenal sudden drop, in orders of magnitude, in their electric conductivity has been attributed to a periodic lattice distortion and a modulation of electron density, paving way for charge density formation in these crystals. For the first time, the formation of characteristically commensurate charge density waves satellite reflections (qCDW = 0.3333 c*), dominantly driven by the Cu-atoms' charge ordering and the cooperative Jahn-Teller distortions on DCNQI molecules, was modelled and analysed.

Tantalum diselenide (4Hb-TaSe2) crystals undergo phase transition from a metallic (T > 600 K) to an insulating (T < 600 K) phase. These crystals belong to the layered compounds of transitional metal dichalcogenides, which are famous for their gigantic magneto-resistance, rich phase diagram and polytypic nomenclature. In agreement with the existing experimental data, electron diffraction simulation shows that the phase transition (with Tc = 410 K) in these crystals invokes the formation of hexagram clusters of commensurate charge density wave (CDW) peaks, which surround each Bragg's peak of the high temperature phase. Moreover, these commensurate CDW peaks are rotated by 13.9° relative to the lattice, with a wave vector given as qCDW = 0.277 a*. Two satellite reflection orders are also observed – a unique characteristic of intertwined crystals.

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PhD

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

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