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Theory of photoinduced electron-phonon-coupled dynamics in two-dimensional charge-ordered systems

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Photoexcitations cause phase transitions from different types of insulators to metals in organic compounds. Their ultrafast dynamics are theoretically studied on the basis of electron-phonon-coupled wave functions in extended Holstein-Peierls-Hubbard models on anisotropic triangular lattices. We focus on 2D 1/4-filled-band charge-ordered insulators, \theta-(BEDT-TTF)2RbZn(SCN)4 and \alpha-(BEDT-TTF)2I3, which have similar Coulomb-driven charge orders and quite different photoinduced dynamics.

On picosecond timescales, couplings with inter-molecular lattice phonons are evident. In the \theta compound, the charge order is quickly recovered after photoexcitation because molecular rotations stabilize the charge order in a stripe-by-stripe manner. In the \alpha compound, the charge order is easily melted to create a macroscopic metallic domain because inter-molecular lattice phonons have much weaker effects [1].
On ten-femtosecond timescales, couplings with intra-molecular vibrations are evident. In the \alpha compound, a coherent oscillation of correlated electrons and subsequent Fano destructive interference with intra-molecular vibrations have been observed, which are well reproduced by calculations based on exact many-electron-phonon wave functions [2].

[1] Y. Tanaka and K. Yonemitsu, JPSJ 79, 034708 (2010).
[2] Y. Kawakami et al., PRL 105, 246402 (2010).

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