

# Coherent Phonon Wavepackets in Quasi-1D Organic Molecular Crystals

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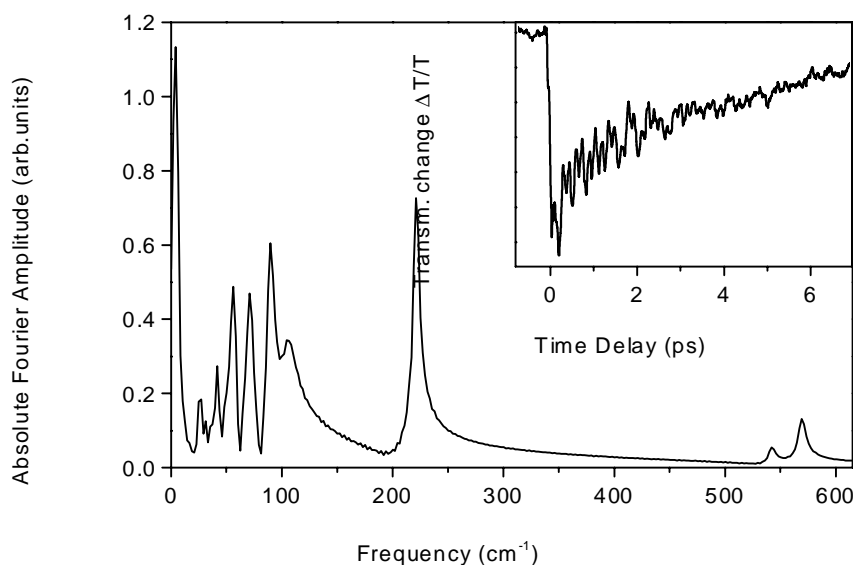
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Organic thin films with semiconducting properties have recently attracted large interest due to novel device possibilities like organic LED, lasers, and solar cells. Particularly attractive for applications are molecules which form quasi-1D crystals: Here, the strong orbital overlap between neighboring molecules favors the generation and transport of charge carriers. However, the *phonon properties* of such 1D organic crystals, related to e.g. *exciton self-trapping*, might be critical for the realization of emission devices. Therefore, a detailed investigation of the exciton-phonon interaction in these materials, having a rich variety of vibronic excitations, is required.

We have time resolved the *coherent motion of external and internal phonons* in thin films of MePTCDI (N-N'-dimethylperylene-3,4,9,10-dicarboximide), employed as a model system for a quasi-1D organic molecular crystal [1]. In the experiment, the phonon modes coupled to the excitonic transition are impulsively excited using 25fs pump pulses, creating phonon wave packets which oscillate at the characteristic frequencies of the material. This propagation of the phonon wave packets is measured as a transmission modulation by a probe pulse (Fig. 1, inset). The Fourier spectrum reveals oscillations at *eleven different frequencies*, see Fig. 1.

We show that the three coherent oscillations with highest frequencies are due to intramolecular vibrations and that the six oscillations following towards lower energy stem from lattice phonons. This interpretation is based on symmetry considerations, density-functional tight-binding calculations [2] of the vibrational energies of the isolated MePTCDI molecule and on a comparison with literature data. In addition, we will discuss the experimentally determined damping times of the external modes, which show a systematic decrease with increasing phonon energy.



Absolute of the complex Fourier amplitude of the fitted oscillatory contribution to the experimental differential transmission signal (shown as inset). The three highest energetic modes stem from intramolecular  $A_g$  vibrations, the six modes between 33 and 105  $\text{cm}^{-1}$  from librational lattice phonons and the two lowest energetic modes at 5 and 25  $\text{cm}^{-1}$  are due to intramolecular  $B_g$  modes.

[1] T. Hasche, T.W. Canzler, R. Scholz, M. Hoffmann, K. Schmidt, Th. Frauenheim, and K. Leo, Phys. Rev. Lett., accepted for publication.

[2] R. Scholz et al., Phys. Rev. **B 61**, 13659 (2000).