Coherent exciton-vibrational dynamics and energy transfer in conjugated organics

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In a new theoretical study described in a *Nature Communications* paper, Los Alamos scientists demonstrate the appearance of coherent electron-vibrational dynamics after so-called non-radiative relaxation when instead of emitting as light, electronic energy is transferred to vibrations or heat in an unexpected fashion. Understanding this phenomenon is important when designing carrier transport in optoelectronic materials.

The production of vibrations or heat leads to changes in the spatial localization patterns in the excited electrons modulated by vibrational excitations. The effect appears as a 'sloshing' of electron density back and forth between molecular sites. The team shows that this phenomenon is ubiquitous in complex natural and man-made systems, and can help in manipulating excited state dynamics and to improve transfer of energy and charge fluxes in functional materials.

Coherent electron-vibrational dynamics

In the quantum world, coherence in the evolution of the wavefunction—the mathematical description of a quantum system—underpins quantum information processing and operation of quantum computing. In materials science, coherent dynamics of electrons and vibrations may refine the efficiency of energy and charge transport in emerging optoelectronic technologies such as thin film photovoltaics, molecular electronics and energy storage.

The simple model proposed in the paper explains the appearance of coherent exciton-vibrational dynamics due to non-adiabatic transitions, which is universal across multiple molecular systems. The observed relationships between electronic wavefunctions and the resulting functionalities allows us to understand, and potentially manipulate, excited state dynamics and energy transfer in molecular materials.

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