Researchers find conformational disorder tuning charge carrier mobility in 2-D perovskites

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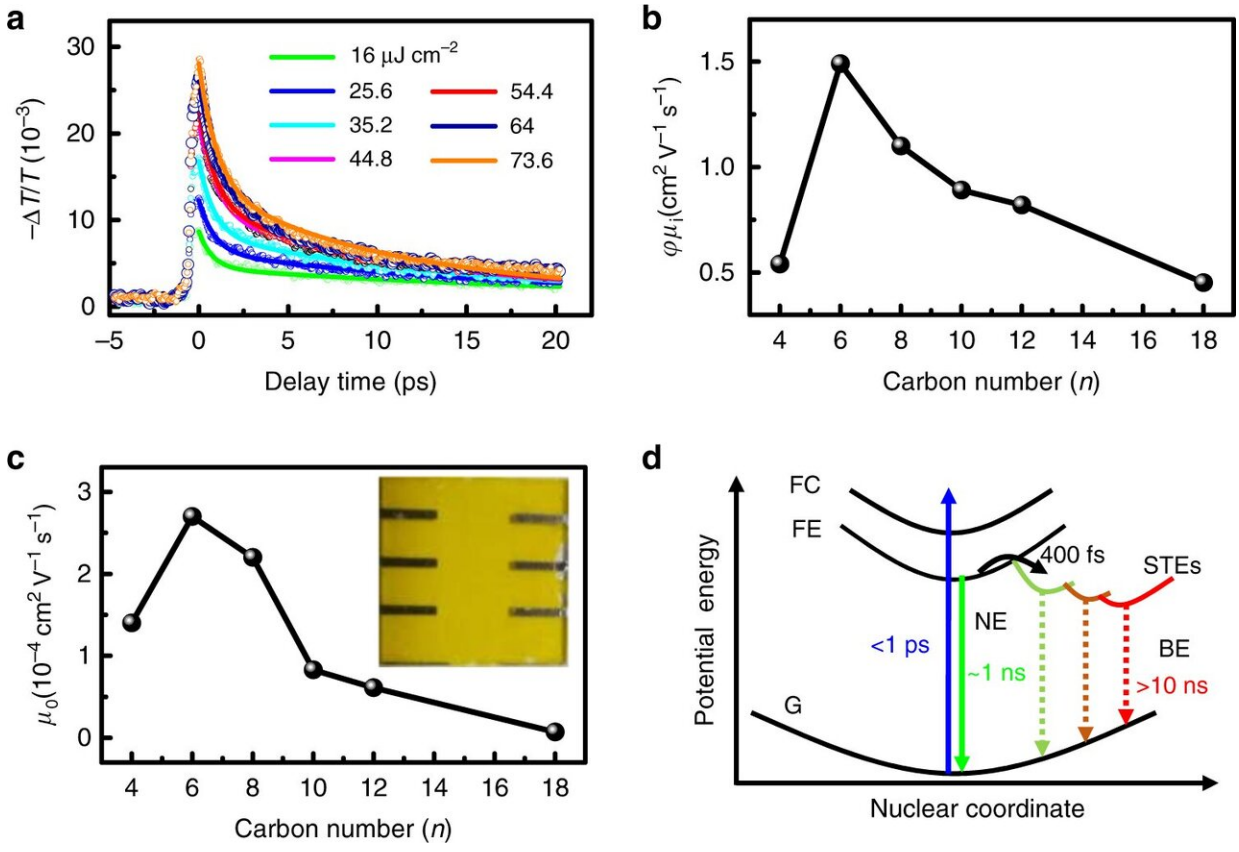

Representative transient THz transmission changes, ΔT/T, of HA2PbI4 (n = 6) for different excitation fluences (λpump = 400 nm). Symbols represent experimental data while solid lines are fitting to the data using biexponential function. b Effective charge-carrier mobility along the film plane (φμi) determined by OPTPS with the pump fluence of 25.6 μJ cm−2. c Out-of-plane charge-carrier mobility (μo) determined by Mott–Gurney analysis of the I–V

data curves. Inset shows a picture of the devices/films. d Schematic of the adiabatic potential energy curves of the ground state (G), free-exciton state (FE), free-carrier state (FC), and various self-trapped excited states (STEs). The vertical dashed line shows possible nonradiative decay processes of the FE and STEs. From: Conformational disorder of organic cations tunes the charge carrier mobility in two-dimensional organic-inorganic perovskites

The organic-inorganic hybrid perovskites (OIHPs) have a multiple application on solar cells, lighting-emitting diodes (LEDs), field effect transistors (FETs) and photodetectors. Among the parameters valuing the power conversion efficiency (PCE) of devices based on perovskite materials, the mobility of carriers undoubtedly captures a high weight.

Although researchers have made massive progress by introducing new components into the structure to control the mobility of the carriers, the understanding on the atom level about how the component affects the performance is still unknown.

To solve the problem, the research team led by Prof. Luo Yi and Prof. Ye Shuji from the University of Science and Technology of China (USTC) of the Chinese Academy of Sciences (CAS) synthesized a series of 2-D OHIPs films with large organic spacer cations.

By a sequence of measurements, including sum frequency generation vibrational spectroscopy (SFG-VS), optical-pump terahertz-probe spectroscopy (OPTPS), current voltage (I-V) measurements, temperature-dependent PL spectroscopy and X-ray diffraction (XRD) measurements, the researchers found the correlation among the conformation of the organic cations, the charge-carrier mobility and broadband emission.

Mobility and broadband emission showed strong dependence on the

molecular conformational order of organic cations. The gauche defect and local chain distortion of organic cations are the structural origin of the in-plane mobility reduction and broad emission in 2-D OIHP films. The interlayer distance and the conformational order of the organic cations co-regulate the out-of-plane mobility.

The result was published in *Nature Communications* on Oct. 30.

This work provides a physical understanding of the important role of organic cation conformation in optimizing the optoelectronic properties of 2-D OIHPs, revealing the structure-property relationship in the perovskite research at the molecular level.

More information: Chuanzhao Li et al. Conformational disorder of organic cations tunes the charge carrier mobility in two-dimensional organic-inorganic perovskites, *Nature Communications* (2020). DOI: 10.1038/s41467-020-19330-7

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