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Self-Trapped Exciton Diffusion in a Lead-Free Two-Dimensional Hybrid Perovskite

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Abstract

Lead halide perovskites have demonstrated the potential of main-group metal halide materials as promising candidates for next-generation optoelectronic applications, including solar cells, LEDs, lasers, sensors, and photocatalysis. In many of these materials, light emission is coupled to self-trapped excitons (STEs), where excitation causes an elastic lattice distortion forming a trapping potential for excitons. Although STEs are typically considered immobile, exciton diffusion plays a crucial role for optoelectronic applications.

We investigate the optical properties and exciton dynamics of the lead-free hybrid perovskite $[CMA]_4[Bi_2Cl_{10}]\cdot H_2O$ (CMA = cyclohexylmethylammonium). The material features a wide band gap of 3.5 eV and broad photoluminescence centered at 2.0 eV (FWHM ≈ 0.5 eV). This white-light emission is attributed to STE formation, driven by strong electron–phonon coupling. Using temperature-dependent, time-resolved, and spatially resolved photoluminescence spectroscopy, we reveal an unexpected regime of diffusive STE transport, with diffusion coefficients on the order of 0.1 cm^2/s. Remarkably, the diffusion accelerates with increasing temperature, leading to diffusion lengths exceeding 1 μm, facilitated by long carrier lifetimes of up to 400 ns.

These results constitute the first evidence of STE diffusion in a two-dimensional hybrid perovskite, challenging the prevailing notion of STEs as localized and immobile. Our findings offer new insights into exciton transport mechanisms and emission helping design guidelines for future optoelectronic perovskites devices.