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# Postsynthesis Spontaneous Coalescence of Mixed-Halide Perovskite Nanocubes into Phase-Stable Single-Crystalline Uniform Luminescent Nanowires

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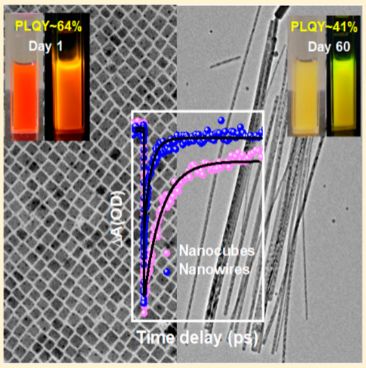
*Supporting Information*

**ABSTRACT:** All inorganic mixed-halide perovskite, $CsPb(Br_xI_{1-x})_3$ ($0 \leq x \leq 1$), nanocrystals possess tunable photoluminescence with high quantum yield in the visible window. However, the photoluminescence degrades rapidly with postsynthetic aging due to the spontaneous ion separation and phase instability. Here we show that the postsynthetic aging of $CsPb(Br_xI_{1-x})_3$ nanocubes spontaneously forms highly uniform single-crystalline nanowires with a diameter of 9 ± 0.5 nm and length of up to several micrometers. The nanowires show bright photoluminescence with an absolute photoluminescence quantum yield of 41%. Rietveld refinement identifies the stable orthorhombic phase of the nanowires, implying a phase transition from the cubic crystallographic phase of the nanocubes during the morphology evolution. Transient absorption spectroscopy reveals a faster excited-state decay dynamic with a large exciton delocalization length in 1D nanowires. Our findings elucidate the insights into the postsynthesis morphology evolution of mixed-halide perovskite nanocrystals leading to luminescent nanowires with excellent crystal phase stability for potential optoelectronic applications.



All-inorganic cesium lead halide perovskite ($CsPbX_3$, X = Cl, Br, I) nanocrystals (NCs) are at the center of current research owing to a range of potential applications in solar cells, light-emitting diodes, photodetectors, and lasers.[1−5] Remarkably high photoluminescence quantum yield (PLQY) has been obtained from $CsPbBr_3$, which leads to the fabrication of efficient light-emitting diodes.[6,7] Complementarily, high carrier mobility, large diffusion length, and ultrafast interfacial charge transfer make $CsPbBr_3$ an attractive candidate for solar cell fabrication.[2,4,5,8−10] Inspiring power conversion efficiency was obtained from $CsPbBr_3$; however, a relatively large band gap (2.36 eV) limits $CsPbBr_3$-based photovoltaic devices.[11] Specifically, $CsPbI_3$, with a narrower band gap (1.73 eV), has shown high solar power conversion efficiency over 17%.[1,12] The cubic crystallographic phase of $CsPbBr_3$ is energetically stable, exhibiting the highest PLQY.[6] On the contrary, cubic $CsPbI_3$ is thermodynamically unstable because it converts into the nonphotoactive yellow orthorhombic nonperovskite phase with a larger band gap (3.0 eV) at room temperature.[11,13,14] Such a crystal phase instability is detrimental for photovoltaic applications because the orthorhombic phase tends to form during film annealing or upon exposure to ambient conditions.[11,15] Strategies to address the phase stability issue involve alloying with halide ions or using suitable ligands and cations to stabilize the cubic phase.[9,16−18] The partial substitution of bulky $I^-$ with the relatively smaller sized $Br^-$ results in stable $CsPb(Br_xI_{1-x})_3$ structures that are thermodynamically stable at room temperature.[18,19] Such mixed-halide composition is attractive because the band gap can be controlled by adjusting the ratio of halide ions.[6,18] However, mixed-halide perovskites were often reported to be phase-segregated into iodide- and bromide-rich phases, which leads to charge-carrier trapping into the iodide-rich regions.[18,20] Hence, the reported literature on the mixed-halide $CsPb(Br_xI_{1-x})_3$ perovskites is counterintuitive and highly depends on the synthesis protocols. Herein we report for the first time on the in situ formation of phase-stable homogeneous mixed-halide $CsPb(Br_xI_{1-x})_3$ ($x = 0.5$, CPBI) luminescent nanowires (NWs) of several micrometers length through the spontaneous coalescence of nanocubes under

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