Supporting information for

Highly efficient copper-based halides single crystals with violet emission for visible light communication

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Experimental section

Materials: Potassium bromide (KBr, 99.99%, Sigma-Aldrich), Cuprous Bromide (CuBr, 99.0%, Sigma-Aldrich), Hydrobromic acid (HBr, Adamas, 48 wt.% in water), Hypophosphorous acid (H_3PO_2, Adamas, 50 wt.% in water), Isopropanol (C_3H_8O, Greagent, 99.7%).

Synthesis of K_2CuBr_3 single crystals

K_2CuBr_3 single crystals were prepared via a cooling-induced crystallization method. 2.38 g KBr and 1.43g CuBr powders were first dissolved in 2 mL HBr, 2 mL H_2O and 0.2 mL H_3PO_2 in a glass bottle at 100 ℃. Then, the mixture solutions were filtered by a 0.22 μm filter. Following this, the temperature was slowlly reduced to room temperature at a rate of 1 ℃/h. Finally, the obtained crystals were washed with isopropanol and dried in the vacuum at room temperature.

Characterizations

XRD spectrum was recorded using a Cu Kα radiation (XRD-6100, SHIMADZU, Japan). Optical characterizations were collected by a

spectrofluorometer (Edinburgh Instruments Ltd., FLS1000, United Kingdom). XPS spectra of the samples were obtained by using an ESCA Lab220I-XL. Thermogravimetric spectrum was recorded using a TGA2 equipment (Mettler Toledo, Switzerland). SEM images were captured by a Quattro S system equipped with an energy dispersive spectrometer.

Measurement of visible light communication

The VLC setup is shown in Figure 5a, where the AC signal is generated by an arbitrary waveform generator (AWG, Tektronix AFG31102), which is combined with a 6.2V DC bias via a bias-T (Mini-Circuits Bias-Tee ZFBT-6GW+) to drive the LED. A -3dB bandwidth photodetector (PD, Thorlabs PDA36A2) at 20 MHz was used to convert the optical signal to an electrical signal. The obtained electrical signals were further sampled by a digital storage oscilloscope (DSO, LeCroy WaveSurfer 432) and processed offline by MATLAB.

DFT calculations

The electronic band structure of K_2CuBr_3 was calculated using the open source CP2K package with double-zeta basis sets (DZVP-MOLOPT) and Goedecker–Teter–Hutter pseudopotentials.[1,2] An energy cut-off 400 Ry was used and the structure was relaxed until the maximum geometry change and maximum force less than 3×10^{-3} and 4.5×10^{-4} Hatree/Å. The electronic band structure was calculated at the theoretical level of HSE06 and the auxiliary density matrix method (ADMM) was used to accelerate the convergence. Online open source tool seek-path was used to generate the high-symmetry points along the first Brillouin zone,[3] and the open source code Multiwfn was used to extract the density of states (DOS) from the molden file exported by CP2K.[4]

Reference

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