Electronic Supplementary Information

Controllable fabrication of well-shaped PMBA@CsPbBr₃

nanoparticles for highly sensitive HCl and HBr detection

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Experimental Section

Materials

N, N' -methylenebis(acrylamide) (MBA, 99.0%, AR grade), Caesium carbonate (Cs₂CO₃, 99.0%, AR grade), Lead (II) bromide (PbBr₂, 99.0%, AR grade), toluene (99.5%), N, N'-dimethyl formamide (DMF, 99.9%, AR grade), azobisisobutyronitrile (AIBN, 98%), 4-cyano-4-(thiobenzoyl)pentanoic acid (CPADB). All the reagents are directly used without further purification.

Synthesis of PMBA@CsPbBr3 NPs

Firstly, toluene (10 mL) and DMF (0.15 ml) were mixed in a reaction flask with MBA (80 mg), PbBr₂ (7.0 mg) and Cs₂CO₃ (2.9 mg). The flask was sealed and stirred (600 rpm) at room temperature for 72 hours. After that, a mixture of initiator AIBN (2 mg) and chain transfer agent CPADB (5 mg) was injected into the solution. The flask was sealed and stirred (0-1000 rpm) at 80 °C for 0-5 hours. The product was then centrifuged and washed with hexane for three times. The powder was then dried in a vacuum oven for 24 hours. Finally, the PMBA@CsPbBr₃ NPs were obtained.

Detection of acid gases by PMBA@CsPbBr₃

To investigate the sensing properties of PMBA@CsPbBr₃ NPs to acidic gas HCl or HBr, we designed a proof-of-concept experimental device. PMBA@CsPbBr₃ NPs was coated on the platform and equipped with an ultraviolet beam (365 nm) and fiber respectively to excite and record the PL emission from the sample. The gases (HCl and HBr) were controlled from the concentrated solution into a 10 L closed transparent container.

Characterization

JEOL 7800F Field Emission Scanning Electron Microscope was used to test the SEM image. TEM and high-resolution TEM (HR-TEM) characterization are collected at 200 kV using a FEI G_2F_{30} electron microscope equipped with Gatan SC 200 CCD camera. The powder X-ray diffraction (PXRD) analysis of the obtained PMBA@CsPbBr₃ NPs was carried out by Bruker AXS D8 Discovery X-ray diffractometer at the wavelength of Cu K (1.97 Å). X-ray photoelectron spectroscopy

(XPS) was tested by AXIS ULTRA instrument (England, KRATOS ANALYTICAL, Ltd.), which is conducted using the Al mono K α X-ray source (1486.6 eV) at 150 W with the acquisition times of 220 s for chemical element analysis. Ultraviolet and visible absorption (UV-vis) spectra were collected using a Cary 5000 UV-Vis-NIR spectrophotometer. Fluorescence spectra and absolute PLQYs were collected using an integrated sphere on an Edinburgh Instruments FLS920 spectrophotometer.

Stabilities

For environmental stability test, PMBA@CsPbBr₃ NPs were conducted by placing them under atmosphere over time, of which PL intensities were recorded. For photostability stability test, the PMBA@CsPbBr₃ NPs were exposed to UV light irradiation (365 nm, 0.5 W·cm⁻²) at room temperature, before being subjected to further characterization.

Supplementary Figures



Fig. S1 TEM images of the PMBA@CsPbBr₃ at the stirring speed of 200 rpm (a), 1000 rpm (b) and 0 (without stirring) (c), respectively.



Fig. S2 XPS scanning of the PMBA@CsPbBr₃ NPs.



Fig. S3 (a-f) High resolution X-ray photoelectron spectroscopy (XPS) of Br3d, C1s, Cs3d, N1s, O1s and Pb4f of PMBA@CsPbBr₃ NPs.



Fig. S4 PL spectra of the PMBA@CsPbBr₃ NPs exposed to various volatiles.



Fig. S5 PL spectra of the PMBA@CsPbBr3 NPs in HBr atmosphere for different times.



Fig. S6 The photographs of PMBA@CsPbBr₃ NPs for sensing HBr over times.



Fig. S7 TEM (a), HR-TEM (b) and SEM (c) of PMBA@CsPbBr₃ NPs after three sensing cycles. (d) PL spectra of PMBA@CsPbBr₃ NPs at 0, 12 min with HBr gas and heating for 30 min. (e) Cycling tests of PMBA@CsPbBr₃ NPs over different sensing.



Fig. S8 PL spectra of PMBA@CsPbBr3 NPs in HCl atmosphere for different times.



Fig. S9 PL intensities of CsPbBr₃ NCs and PMBA@CsPbBr₃ NPs under air (a) and UV (365 nm) irradiation (b) over time.