Supporting Information

Crystalline borophene quantum dots and their derivative boron nanospheres

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Samples preparation

All of the chemicals were used without purification. First, 50 mg bulk boron powder (99.99 %) was dissolved into 30 mL isopropyl alcohol (IPA) by an ultrasonic concussion to form a clear solution. Then, 20 mg H3BO3 powder (99.998 %) was added into the solution and stirred for 10 h until completely dissolved. Next, 2 mL H2O2 (30 %) solution was dropwise added in the above solution. The resultant solution was vigorously stirred for 5 h at ambient condition. The product was ultrasonically dispersed in 50 mL IPA solution using a high-power probe-type ultrasonic crusher (900 W, 4 s ultrasonication and 6 s pause), and the temperature was always kept at about 5 °C. After 5 h ultrasonication, the product was centrifugated at a speed of 2000 rpm for 1 h and the supernatant was dialyzed. The obtained powder was denoted B-QDs. 5 mg B-QDs powder was ultrasonically dispersed in 30 mL IPA solution, and then different volumes of hydrazine hydrate (HHA) were added into the resultant solution and continued to stir for 5
h. The product was centrifugated at a speed of 10000 rpm for 30 min and the precipitate was washed for three times and dried in a vacuum. Finally, the derivative boron nanospheres (DBS) were prepared. Further, the obtained DBS was calcined at 500 °C for 1 h under argon atmosphere.

**Characterizations**

TEM and HRTEM images were obtained on a JEM–2010F transmission electron microscopy at an accelerating voltage of 200 kV, along with EDX mapping. SEM images were taken using a JSM-7900F field-emission scanning electron microscopy (FE–SEM). The XRD patterns was obtained on a Bruker AXS D8X-ray diffractometer. Raman spectra were recorded on inVia (Renishaw) instrument with a 532 nm Ar-ion laser. XPS measurements were performed on Thermo Fisher Scientific spectrometer using an Al-Kα radiation. Fourier transform infrared (FT-IR) spectra were determined on a Nicolet 6700 FTIR spectrophotometer. The $^{11}$B MAS spectra were detected on a Bruker AVANCE NEO 400 WB spectrometer equipped with a 4 mm standard bore CP MAS probe head whose X channel was tuned to 128.39 MHz for 11B, using a magnetic field of 9.39T at 297 K. The dried and finely powdered samples were packed in the ZrO$_2$ rotor closed with Kel-F cap which were spun at 12 kHz rate. A total of 1000 scans were recorded with 2 s recycle delay for each sample. All $^{11}$B MAS chemical shifts are referenced to the resonances of boron nitride (BN), 99.5% (metals basis) standard (d=0.00). Fluorescence spectroscopy were collected on a Hitachi F4500 fluorescence spectrophotometer. The absorbance was carried out on a Shimadzu UV-2550 UV-vis spectrometer.
Supplementary Figures:

**Fig. S1** A state change of B-QDs solution observed after adding the HHA.

**Fig. S2** TEM images of as-fabricated samples in a similar method (a) except boron powder, (b) except boric acid, and (c) including boron powder and boric acid.

**Fig. S3** The corresponding atomic ratios according to the binding energy shown in Fig. 2g.
Fig. S4 SEM images with different magnifications of the obtained DBS particles.

Fig. S5 (a) Photograph of B-QDs dispersed in IPA solution under ambient light irradiation after 60 days. (b) B-QDs concentration-dependant PL spectra excited by a 325 nm laser. (c) UV-vis spectra of B-QDs with different concentrations. (d) $(ahv)^2$ as a function of $hv$ for band gap determination.
Fig. S6 PL spectra of the B-QDs with different concentrations excited at various wavelengths.