Supporting Information

Oxygen-rich bismuth oxyhalides: Generalized one-pot synthesis, band structures and visible-light photocatalytic properties

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Experimental Section

Materials: Bi_2O_3 was purchased from Aladdin Reagent Co. Ltd. potassium halides (KX, X=Cl, Br, and I) were bought from Tianjin Kermel Chemical Reagent Co. Ltd. BPA was bought from Sinopharm Group Chemical Reagent Co. Ltd. All the chemicals were analytical grade and used as received without further purification and distilled water was used in all experiments.

Preparation: In a typical synthesis, 0.5 mmol Bi_2O_3 were firstly dispersed in 25 mL distilled water by ultrasonic treatment (10 min) and followed by magnetic stirring. Then, 1 mmol KX (X=Cl, Br, or I) was added to and dissolved completely in the solution. After that, 10 ml HNO_3 solution that contain a suitable amount of HNO_3 (see detail in Table 1, by mixing 0.1 M HNO_3 solution with distilled water) was added dropwise into the solution under magnetic stirring condition. The mixture was stirred for another 30 min and then poured into a Teflon-lined stainless-steel autoclave (45 mL capacity) and heated at 160 °C for 12 h. Afterwards, the precipitates were collected by centrifugation, washed several times with distilled water and absolute ethanol, and dried at 60 °C.

Characterization: The crystalline structure of the samples was determined by powder X-ray diffraction (XRD) using a Bruker D8 Advance (Bruker AXS, Germany) X-ray diffractometer with Cu K α. The UV-vis diffuse refection spectra (DRS) were recorded on a UV-vis spectrophotometer (UV-3010, Hitachi, Japan) using $BaSO_4$ as a reference and were converted from reflection to absorbance by the Kubelka-Munk method. The Specific BET surface area was determined by N_2 adsorption-desorption measurements at 77 K in a 3H-2000PS1 (Beijing, China) surface area measurement apparatus.

Computation: The calculations were performed with the Cambridge Serial Total Energy Package (CASTEP) code of Materials Studio based on the density functional theory (DFT). Ultrasoft pseudopotentials are used for the geometry optimization so as to make the computations tractable and efficient. The exchange and correlation interactions were modeled using the generalized gradient approximation (GGA), together with the Perdew–Burke–Ernzerhof (PBE). A plane-wave cutoff energy of 380 eV was employed throughout. Then, the energy and electronic structures were calculated on the basis of the optimized geometry structures.

Photocatalytic measurement: The photocatalytic degradation experiments were carried out in a photochemical reactor (XPA-VII, Nanjing Xujiang Machine-electronic Plant, China), using 1000 W Xe lamp with 420 nm cut-off filter as a light source. All photocatalytic reactions were performed using the same initial conditions: 50 ml of BPA solution (20 mg L^{-1}) was mixed with 50 mg catalyst, under constant magnetic stirring. Prior to irradiation, the solution with the catalyst was stirred for 30 min in the dark to allow the system to reach adsorption equilibrium. After 2 h of irradiation, about 3 mL of the suspension was taken out and the solids were subsequently removed from the solution using a 0.45 μm nitrocellulose filter. Then the BPA content of the solution was determined by UV-vis spectroscopy (UV-1800, Shimadzu, Japan, λ=276 nm).
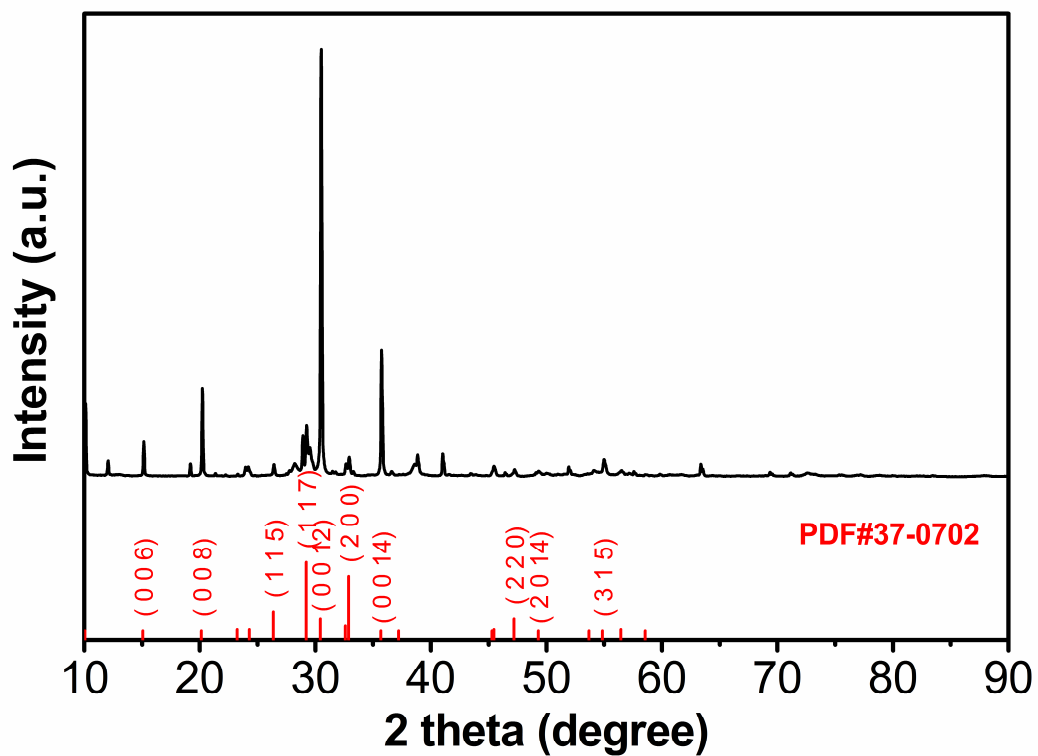
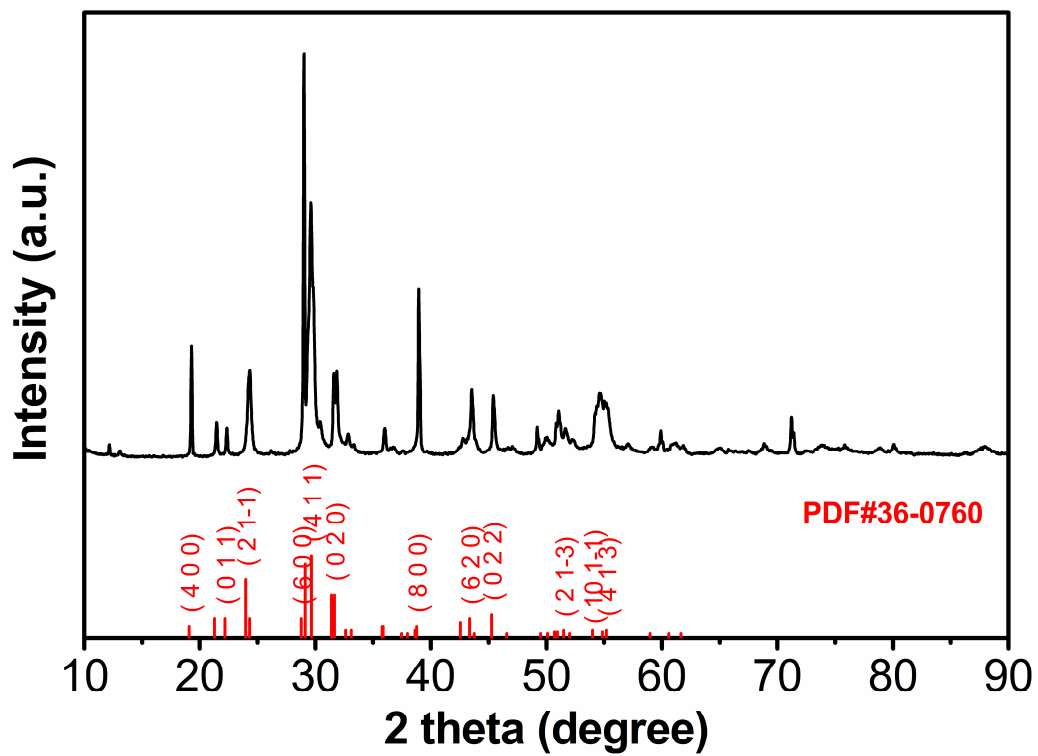Fig. S1 XRD pattern of the as-synthesized sample S1.

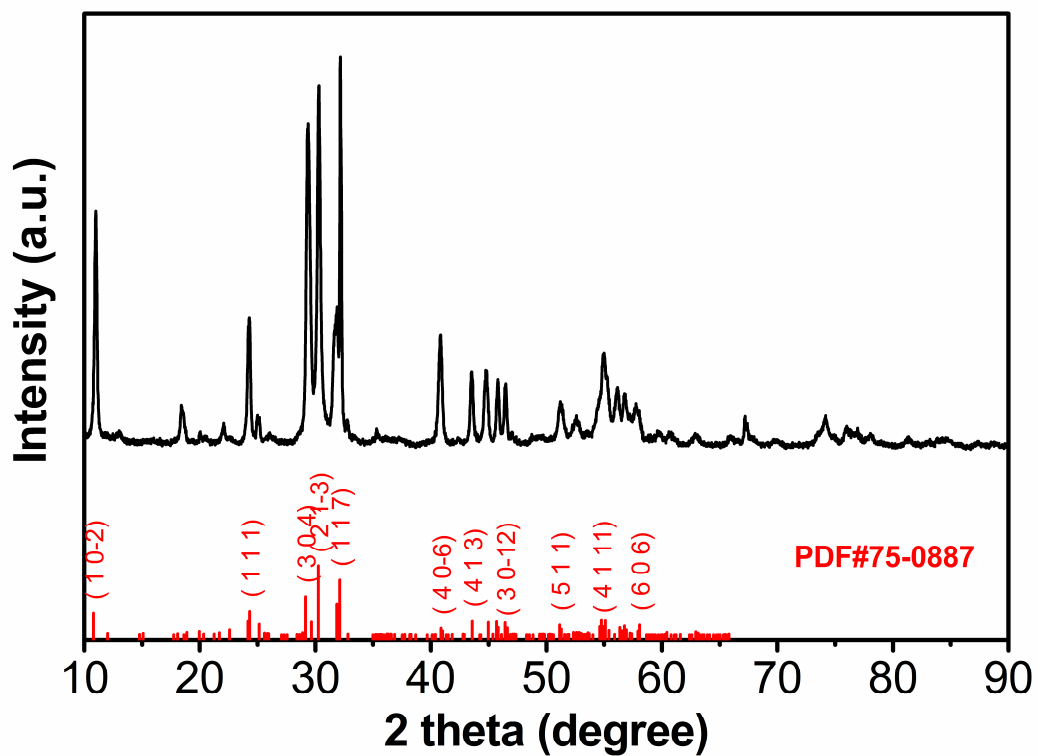Fig. S2 XRD pattern of the as-synthesized sample S2.
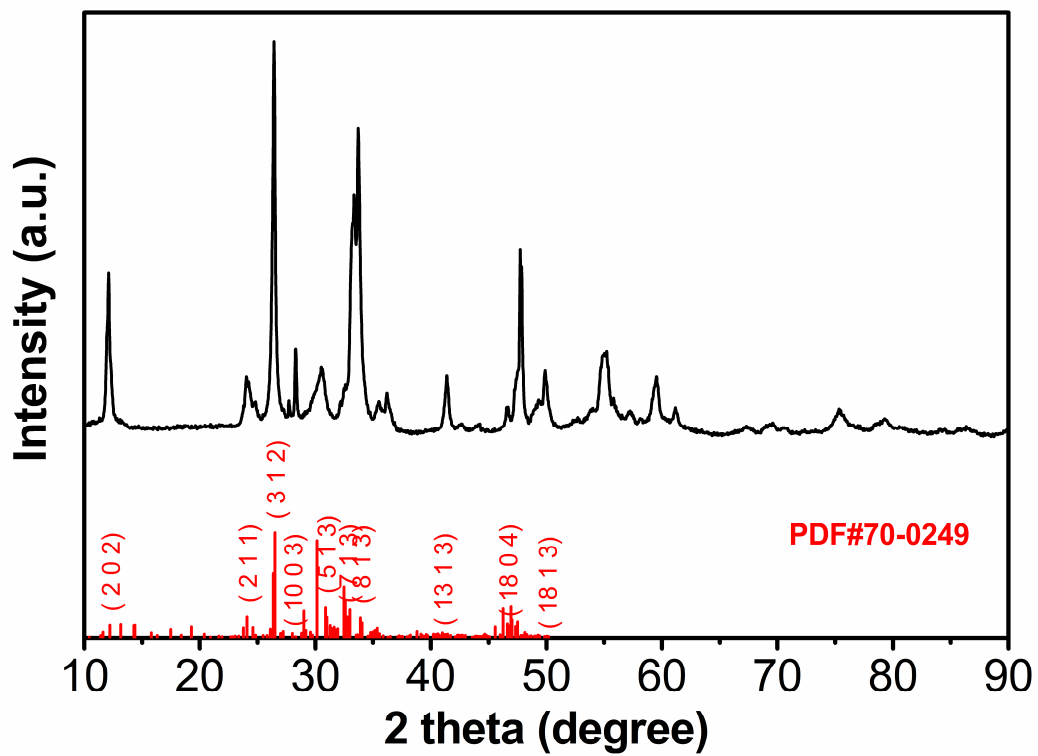
Fig. S3 XRD pattern of the as-synthesized sample S3.

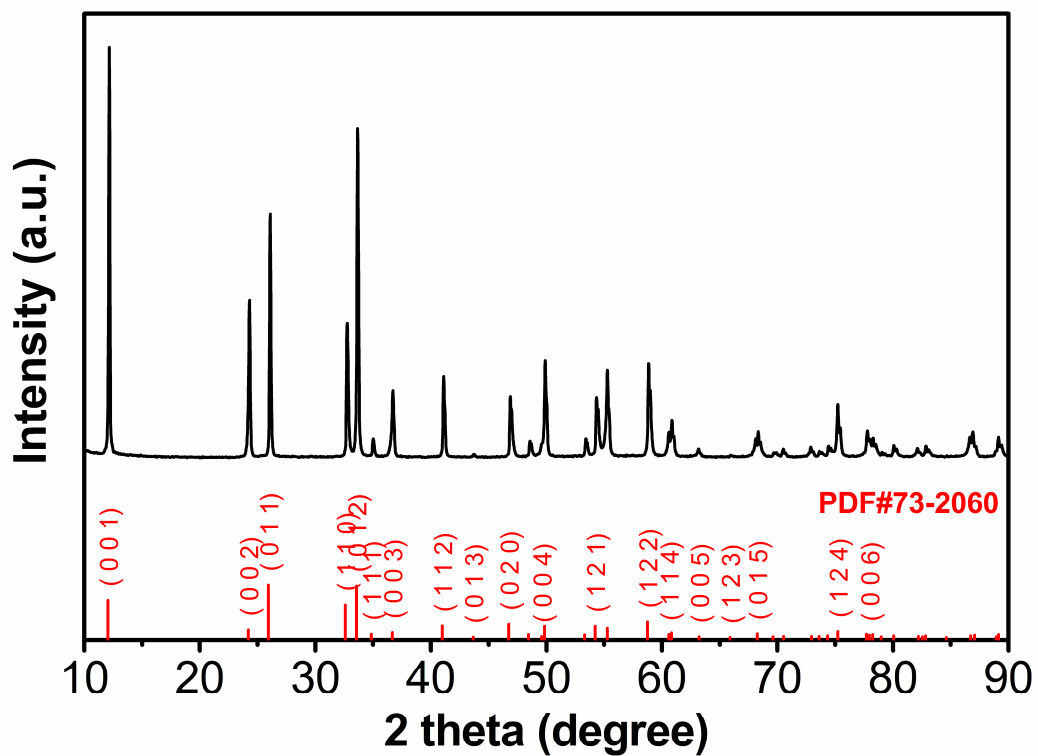Fig. S4 XRD pattern of the as-synthesized sample S4.

5

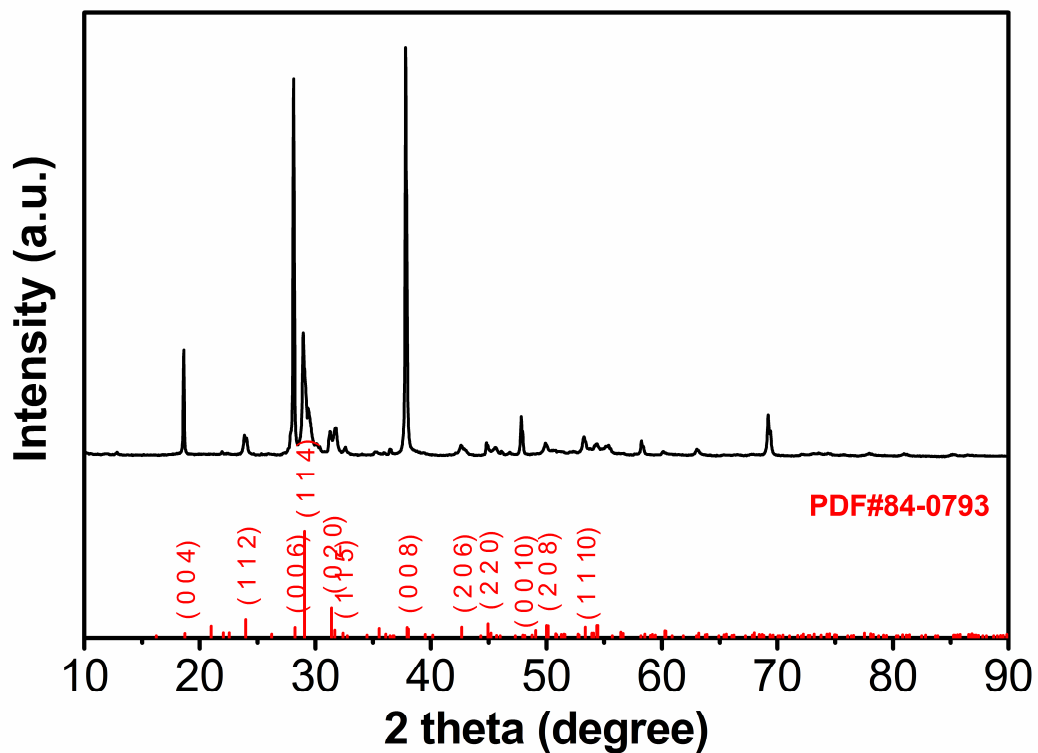Fig. S5 XRD pattern of the as-synthesized sample S5.

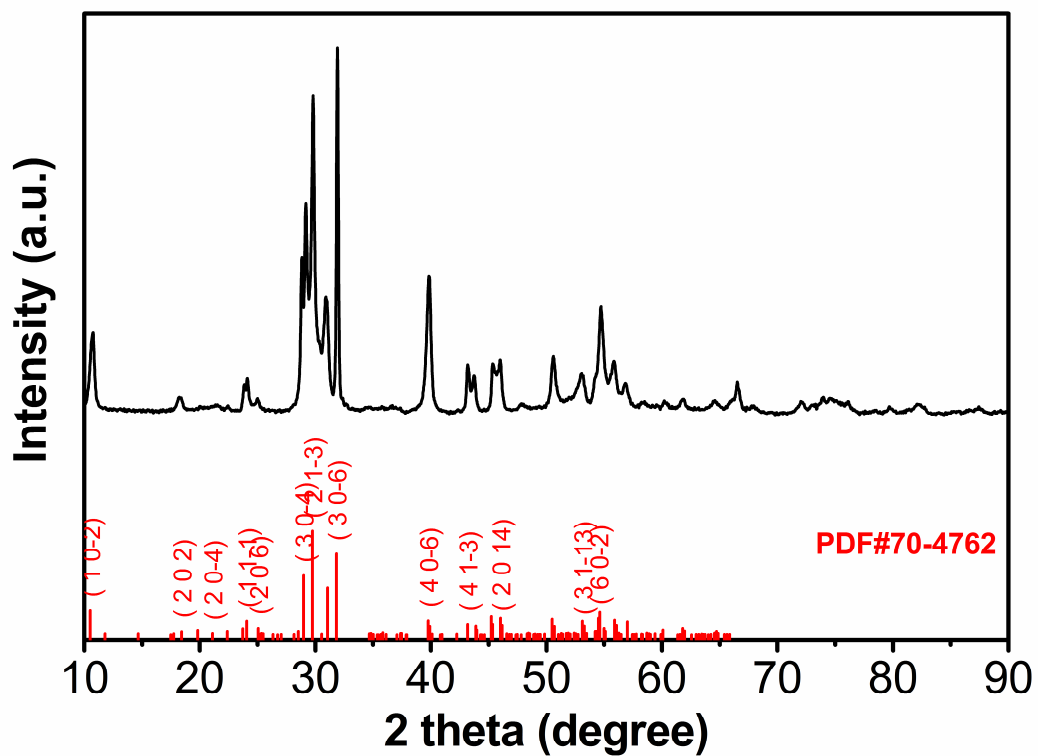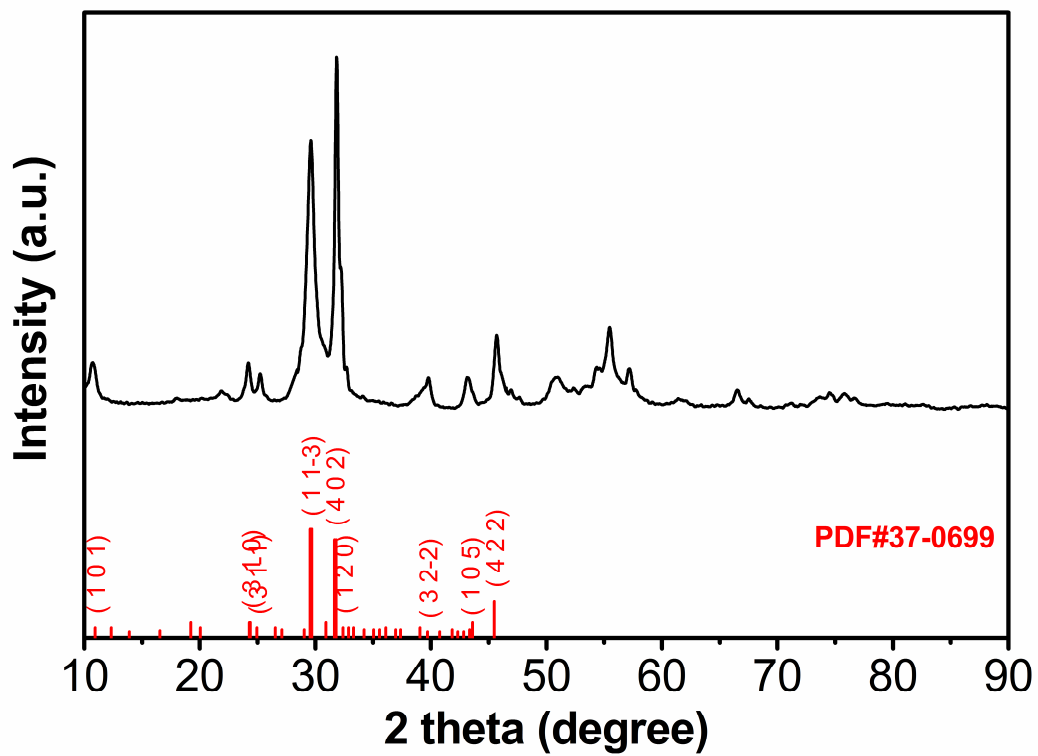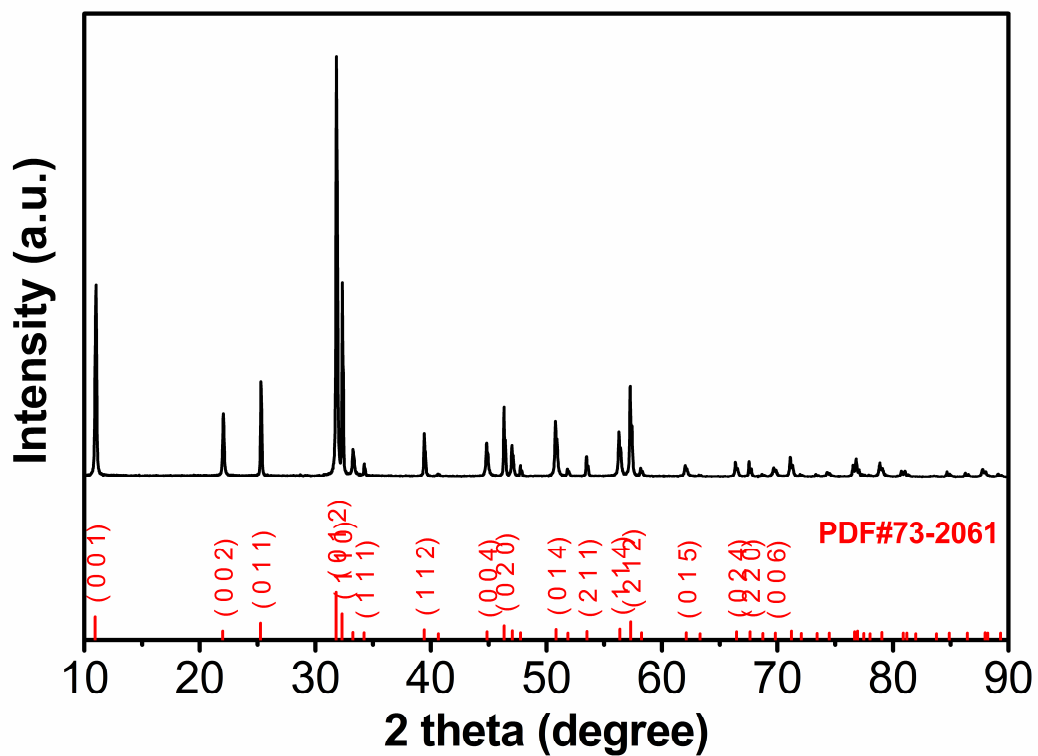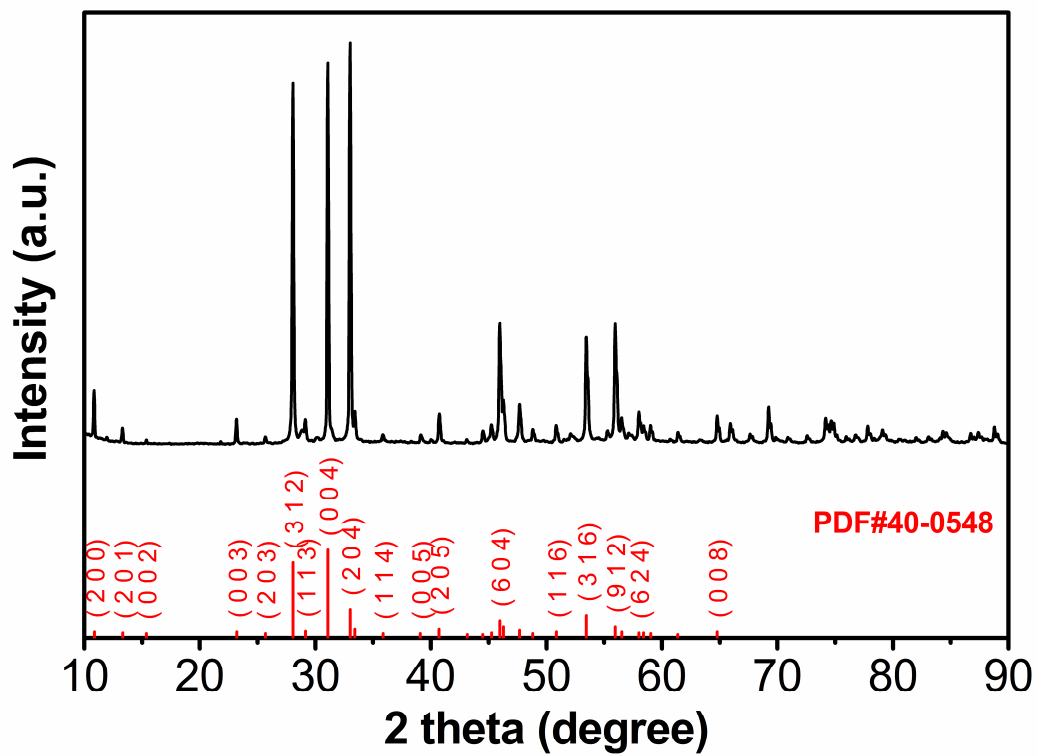Fig. S6 XRD pattern of the as-synthesized sample S6.

6

Fig. S7 XRD pattern of the as-synthesized sample S7.

Fig. S8 XRD pattern of the as-synthesized sample S8.

Fig. S9 XRD pattern of the as-synthesized sample S9.

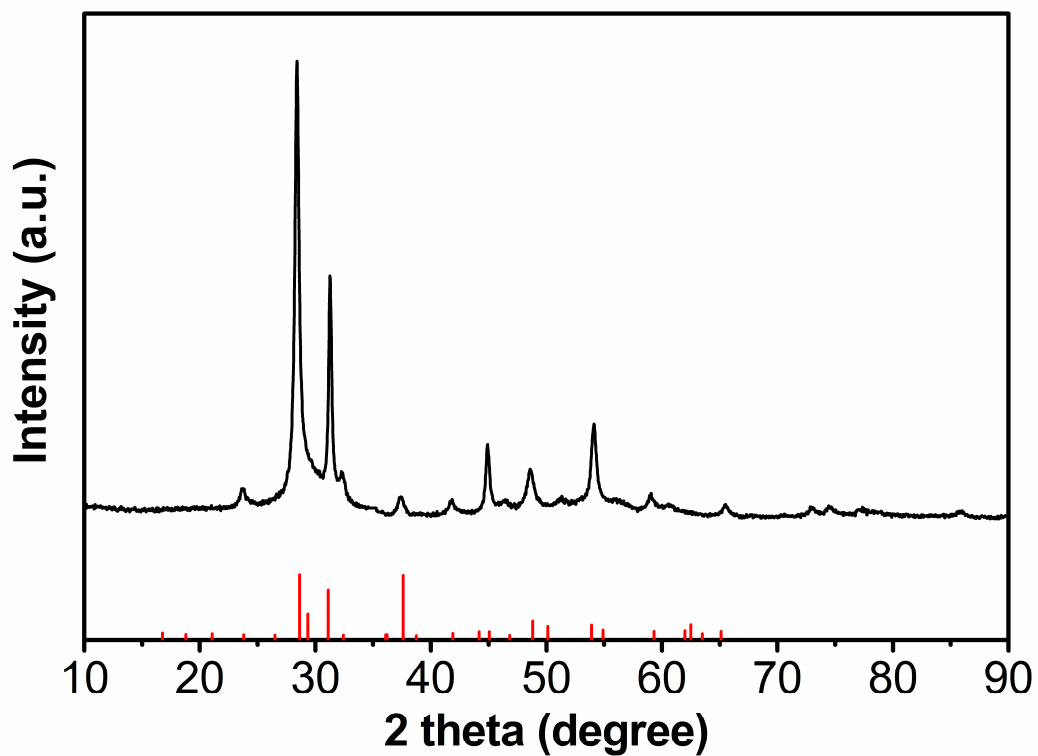Fig. S10 XRD pattern of the as-synthesized sample S10.

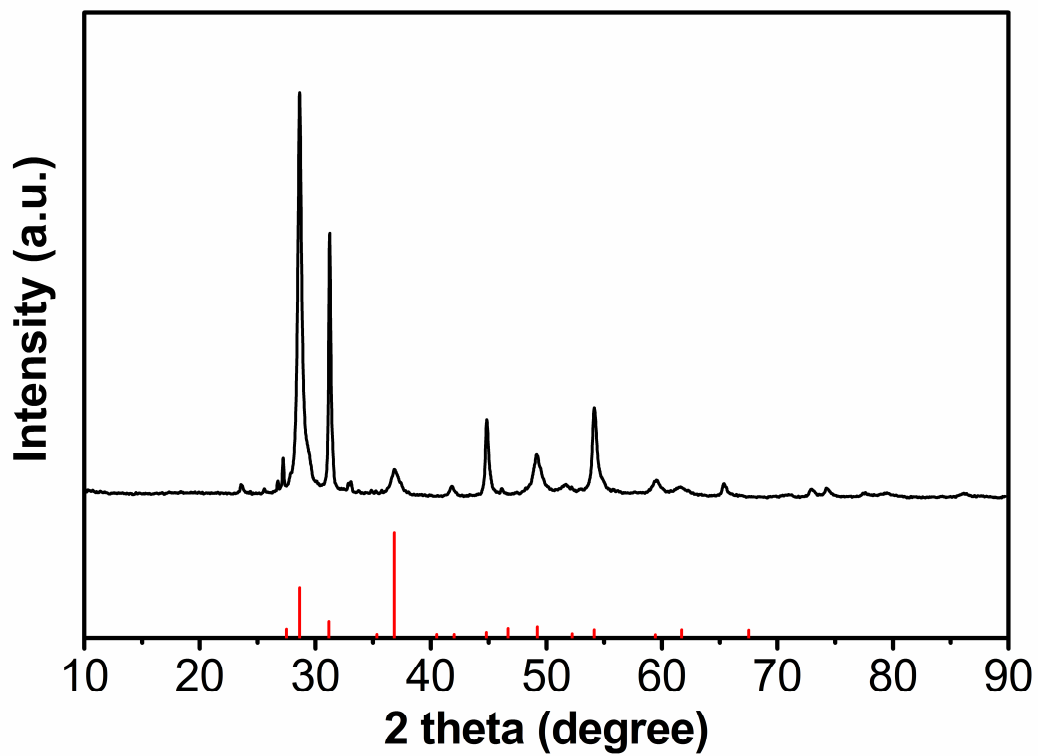Fig. S11 XRD pattern of the as-synthesized sample S11.
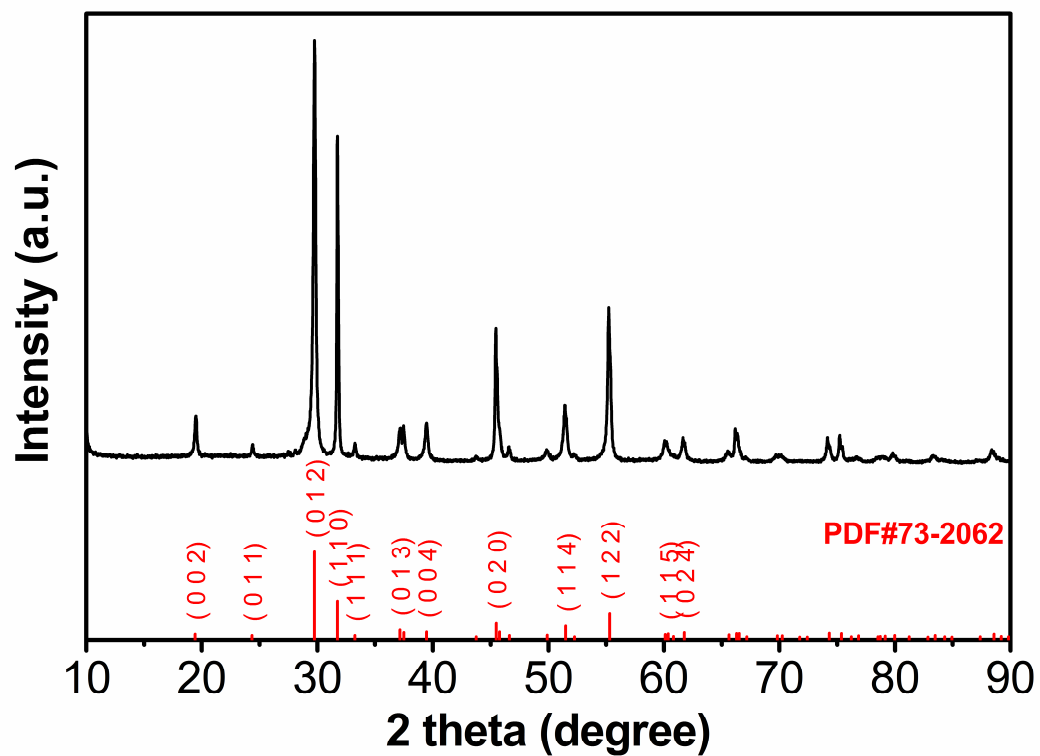

Fig. S12 XRD pattern of the as-synthesized sample S12.

Fig. S13 XRD pattern of the as-synthesized sample S13.