Electronic Supplementary Information

Templated Assembly of $BiFeO_3$ Nanocrystals into 3D Mesoporous Networks for Catalytic Applications

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Table S1. Comparison of catalytic data for *p*-nitrophenol (4-NP) reduction by mesoporous $BiFeO_3$ nanoparticle assemblies (MBFAs) and other reported catalysts from the literature.

Catalyst	**Initial conc. of 4-NP (mmol L^{-1})**	**Conc. of catalyst (mg mL^{-1})**	**Conc. of $NaBH_4$ (mmol L^{-1})**	**Rate constant (s^{-1})**	**Ref.**
Au/Fe_3O_4 NPs	0.18	0.91	7.3	$1.0 \cdot 10^{-2}$	[27]
Au/CuO microstructure	0.081	0.026	32.4	$1.6 \cdot 10^{-2}$	[28]
Cu/Ag NPs	3.3	0.086	333	$0.8 \cdot 10^{-2}$	[29]
Pd/polypyrrole	0.107	0.006	5.9	$0.9 \cdot 10^{-2}$	[30]
Ag/Au dendrites	0.066	0.2	10	$0.6 \cdot 10^{-2}$	[31]
Pd/Ag dendrites	0.066	0.33	10	$3.9 \cdot 10^{-2}$	[32]
Fe_3O_4/graphene/Pt	1.85	1	600	$2.0 \cdot 10^{-2}$	[33]
Fe_3O_4/graphene/Pd	1.85	1	600	$6.1 \cdot 10^{-2}$	[33]
Fe_3O_4/graphene/PtPd	1.85	1	600	$3.7 \cdot 10^{-2}$	[33]
MBFAs	**0.1**	**1**	**5**	$\mathbf{1.8 \cdot 10^{-2}}$	**This work**

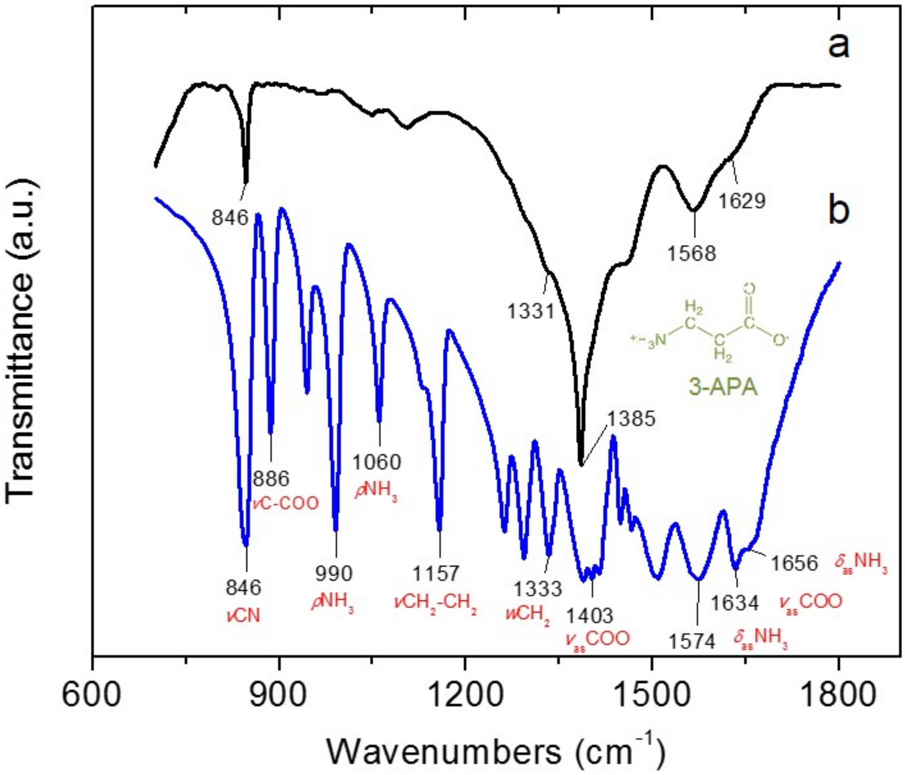

Fig. S1 Infrared spectra for (a) $BiFeO_3$ NPs capped with 3-aminopropanoic acid (3-APA) ligands and (b) pure 3-aminopropanoic acid compound. The assignment of IR peaks of 3-APA to various vibration modes was based on that of ref. [18] (*v* - stretching, *δ* - bending, *w* - wagging, *ρ* - rocking, *s* - symmetric, *as* - asymmetric).

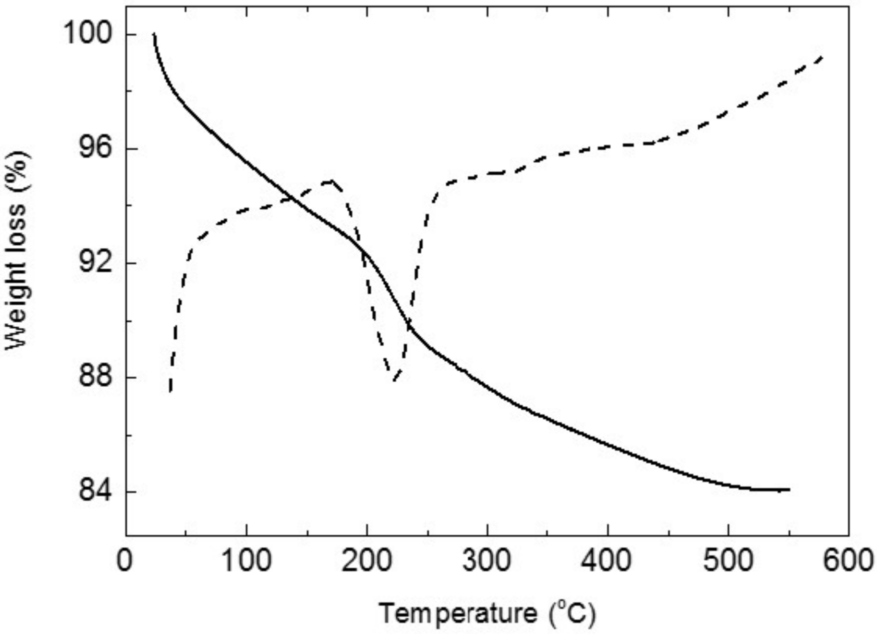

Fig. S2 TG (solid line) and differential thermogravimetric (DTG) (dashed line) profiles of as-prepared $BiFeO_3$ NPs capped with 3-APA showing weight loss of about 7.2% in the temperature range 170–360 °C. This weight loss seems to be accompanied by at least a two-step process as indicated by the DTG curve and corresponds to the decomposition of 3-APA ligand. This process is followed by a gradual weight loss at temperatures between 360 and 530 °C, which correspond to the dehydration and/or dehydroxylation of surface.

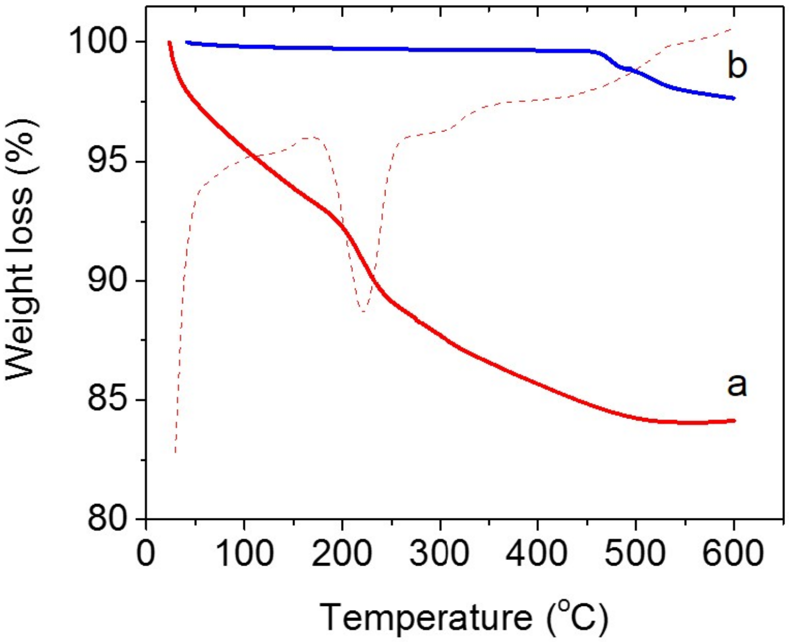

Fig. S3 TG profiles (solid lines) performed in air of (a) as-prepared containing surfactant and (b) mesoporous MBFAs sample. The differential thermogravimetric (DTG) curve (dashed lines) for as-prepared materials is also given.

The TG curve of mesostructured MBFAs sample before calcination shows a weight loss in the temperature range 25–170 °C due to the removal of physisorbed solvent. The weight loss (~9%) observed between 170 and 370 °C, which is accompanied by at least two-step process as indicated by the DTG curve, is attributed to the decomposition of organic matter. This process is followed by a gradual weight loss at temperatures between 370 and 540 °C, which correspond to the dehydration and/or dehydroxylation of surface. The TG curve of mesoporous sample after calcination show a ~1.8% weight loss between 480 and 600 °C, which is attributed mainly to the dehydroxylation of surface –OH groups.

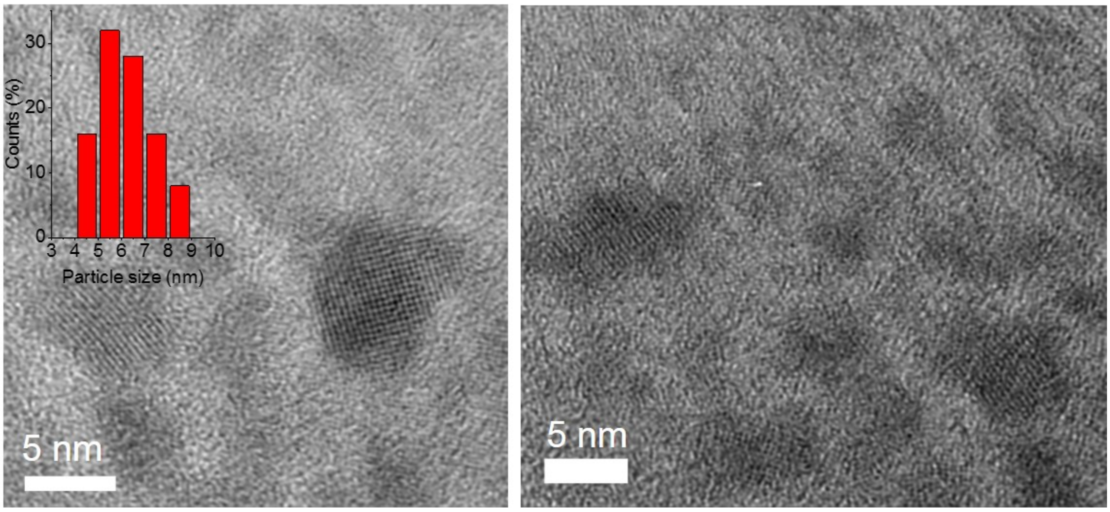

Fig. S4 Typical TEM images of 3-APA–capped $BiFeO_3$ NPs. Inset: the corresponding particle size distribution, indicating an average particle size of 6.2 nm. The particle size distribution was estimated by measuring the size of about 100 individual nanoparticles in several TEM images.

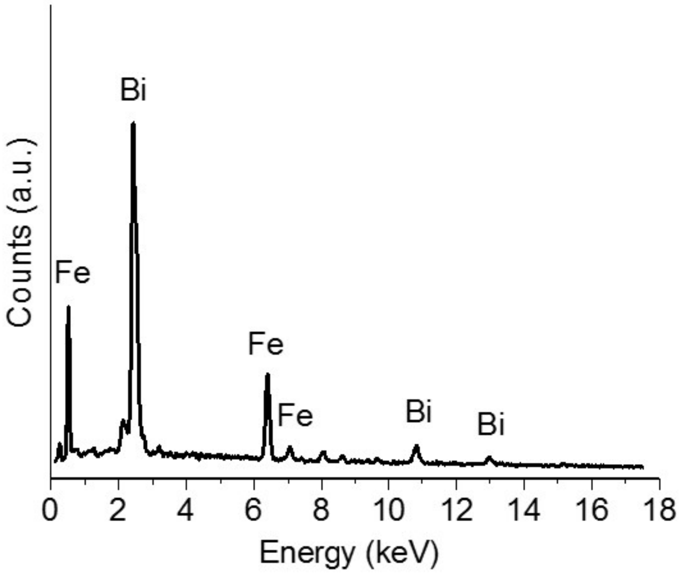

Fig. S5 Typical energy-dispersive X-ray spectroscopy (EDS) spectrum of MBFAs, showing a Bi:Fe atomic ratio of ~1:1.

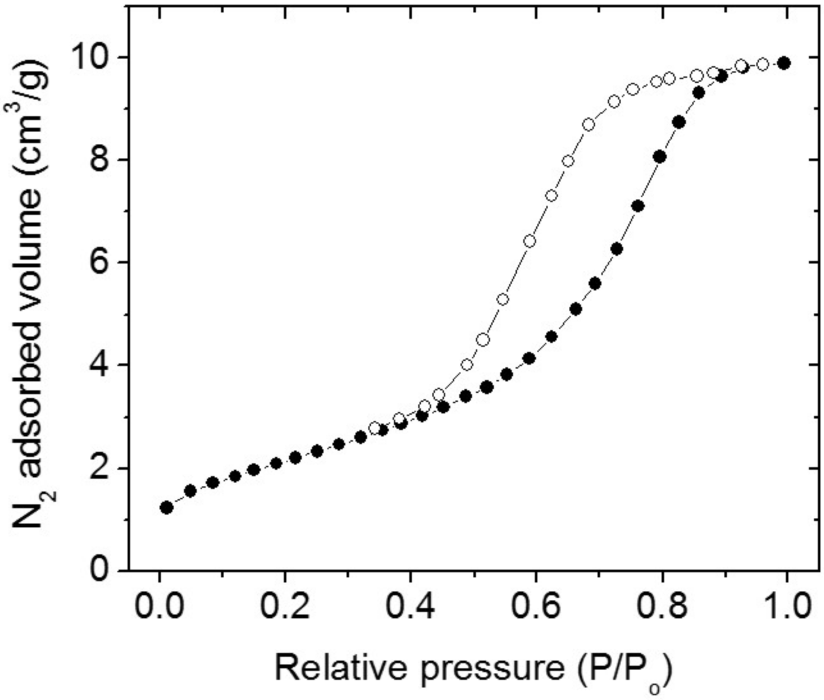

Fig. S6 Nitrogen adsorption–desorption isotherms at 77 K of randomly aggregated $BiFeO_3$ NPs, showing BET surface area of ~8 m^2g^{-1} and total pore volume of ~0.01 cm^3g^{-1}.

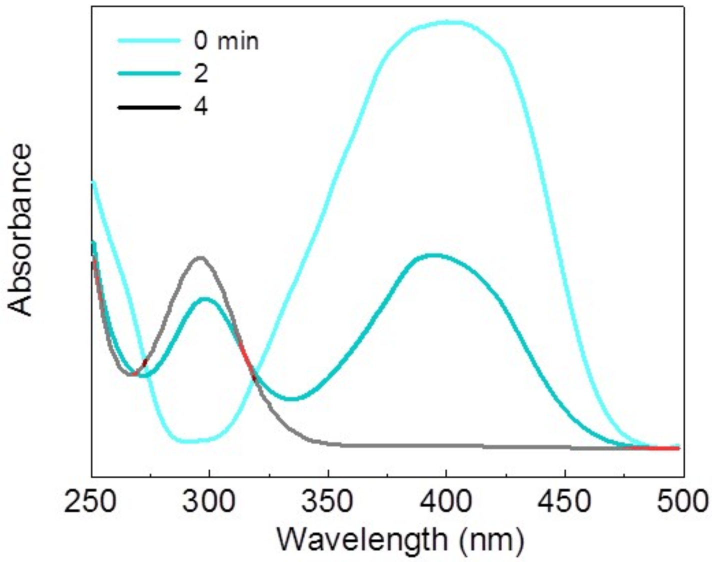

Fig. S7 Time-dependent UV–vis absorption spectra for *p*-nitrophenol reduction by $NaBH_4$ in the presence of MBFAs catalyst.