Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

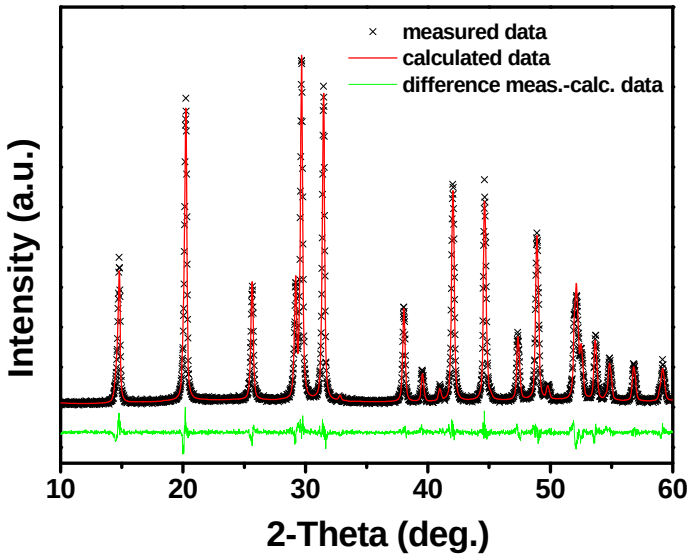

Fig. S1 Rietveld fitting on powder X-ray diffraction data of the as-prepared HP sample (R_{wp}=0.1096, R_p=0.0789, $R_{\text{-blnk}}$=0.0653, and χ^2=1.657).

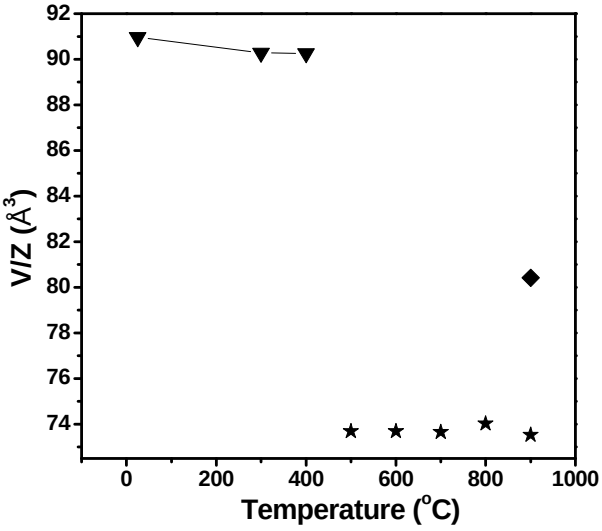

Fig. S2 Unit cell volume dependence of $BiPO_4$ polymorphs on calcination temperature.

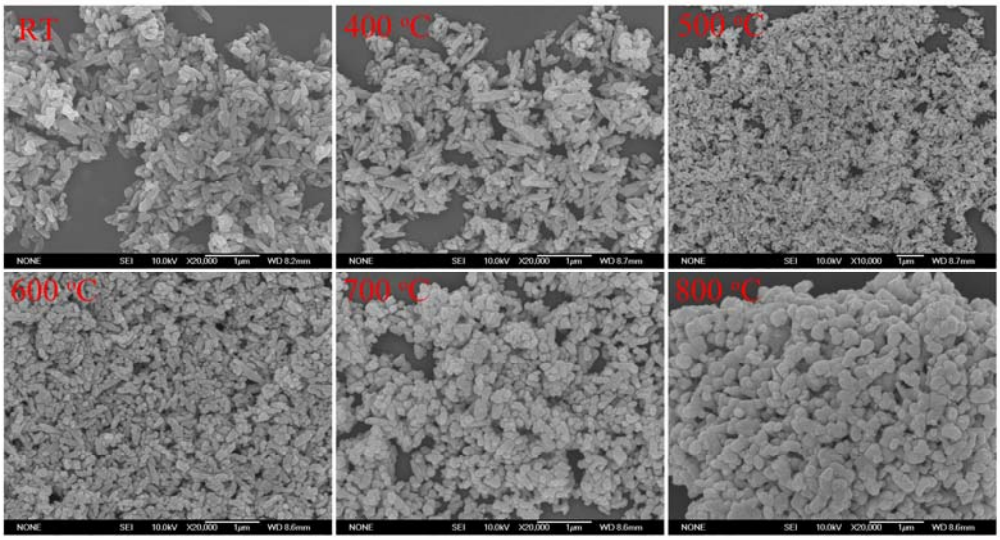

Fig. S3 SEM images of HP and those obtained after calcinations over HP at given temperatures.

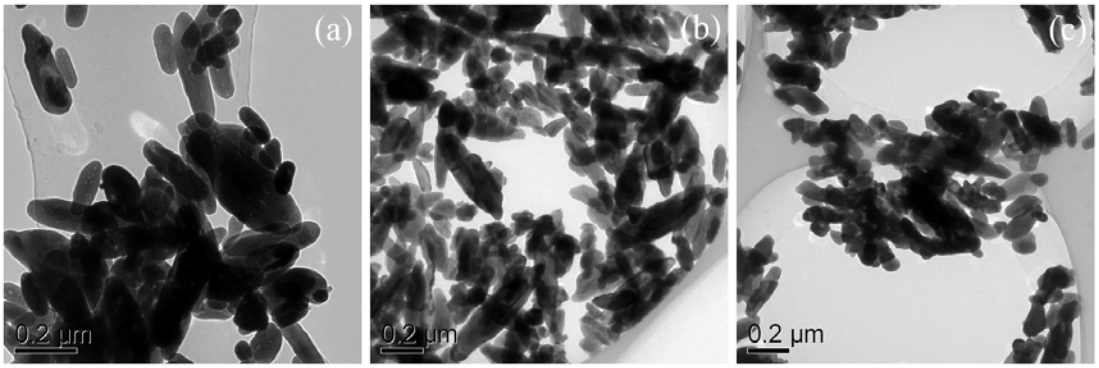

Fig. S4 TEM images of (a) as-prepared HP and those obtained after calcinations over HP (b) at 400 ^{o}C and (c) at 600 ^{o}C.

Table S1 Lattice parameters and atomic positions for HP (RT), LTMP (600 ^{o}C), and HTMP (900 ^{o}C) obtained by Rietveld refinement using GSAS program.

Sample	Lattice parameters	Atom	Site	x	y	z	
HP	$P3_121(152)$	Bi	3b	0.469	0	0.833	R_{wp}=0.1036
	a=6.9597(2)Å	Eu	3b	0.468	0	0.833	R_p=0.0734
	c=6.4551(2) Å	P	3a	0.434	0	0.333	R_{-blnk}=0.0606
	V=270.78(2) Å^3	O1	6c	0.334	0.118	0.451	χ^2=1.482
		O2	6c	0.628	0.114	0.185	
LTMP	$P2_1/n(14)$	Bi	4e	0.286	0.144	0.086	R_{wp}=0.1120
	a=6.7533(3) Å	Eu	4e	0.277	0.155	0.078	R_p=0.0848
	b=6.9404(3) Å	P	4e	0.304	0.155	0.619	R_{-blnk}=0.0767
	c=6.4728(3)Å	O1	4e	0.240	-0.002	0.459	χ^2=1.691
	β=103.717	O2	4e	0.380	0.304	0.514	
	V=294.73(3) Å^3	O3	4e	0.475	0.125	0.806	
		O4	4e	0.123	0.190	0.699	
HTMP	$P2_1/m(11)$	Bi	2e	0.143	0.250	0.168	R_{wp}=0.1082
	a=4.8531(3)Å	Eu	2e	0.111	0.250	0.169	R_p=0.0793
	b=7.0556(4) Å	P	2e	0.378	0.750	0.309	R_{-blnk}=0.0702
	c=4.6881(3) Å	O1	2e	0.669	0.750	0.254	χ^2=1.453
	β=96.199	O2	2e	0.627	0.250	0.169	
	V=159.59(2) Å^3	O3	4f	0.214	0.577	0.177	

Table S2 Bond lengths for HP, LTMP (600 ^{o}C), and HTMP (900 ^{o}C) polymorphs obtained by Rietveld refinement using GSAS program.

HP		LTMP		HTMP	
bond	distance (Å)	bond	distance (Å)	bond	distance (Å)
Bi-O1×2	2.906	Bi-O3	2.458	Bi-O1	2.767
Bi-O2×2	2.534	Bi-O4	2.510	Bi-O2	2.429
Bi-O1×2	2.508	Bi-O1	2.479	Bi-O3×2	2.332
Bi-O1×2	2.476	Bi-O1	2.700	Bi-O3×2	2.547
		Bi-O4	2.504	Bi-O1	2.266
		Bi-O2	2.406	Bi-O2	2.759
		Bi-O2	2.667		
		Bi-O3	2.359		
P-O1×2	1.522	P-O2	1.583	P-O1	1.549
P-O2×2	1.518	P-O3	1.477	P-O3×2	1.540
		P-O4	1.450	P-O2	1.530
		P-O1	1.495		