Electronic Supplementary Information

Structural analysis of α-zirconium phosphate/cerium phosphate/graphene oxide nanocomposites with the flame retardancy to polyvinyl alcohol

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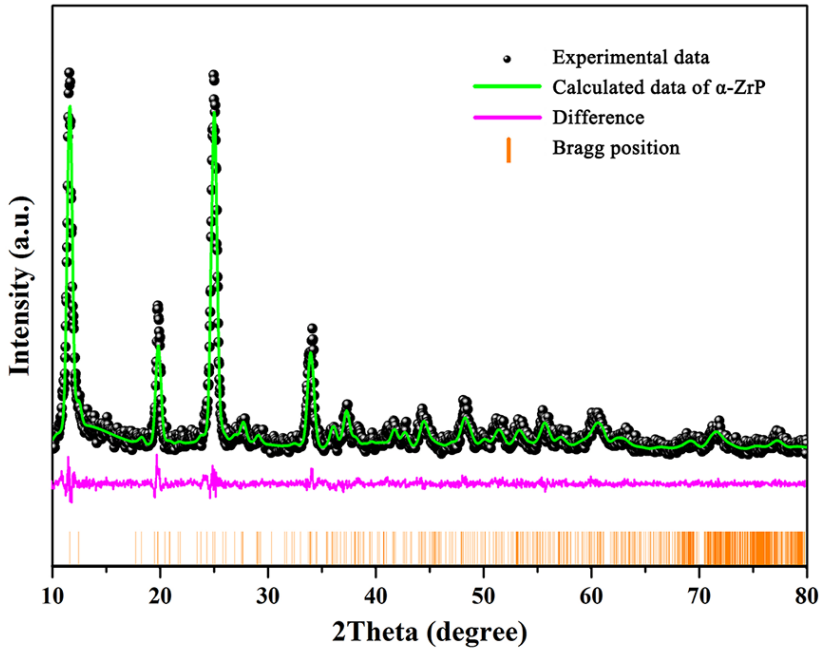

Figure. S1 The Rietveld refinement of pure $Zr(HPO_4)_2·H_2O$.

Table S1 Phase data of pure $Zr(HPO_4)_2·H_2O$.

Formula sum	**$Zr(HPO_4)_2·H_2O$(α-ZrP)**
Crystal system	Monoclinic
Space-group	P 1 21/n 1 (14)
Cell parameters	a=9.110(5) Å b=5.270(4) Å c=15.457(5) Å
Cell ratio	a/b=1.7287 b/c=0.3409 c/a=1.6967
Cell volume	726.54(2) $Å^3$
R factor	R_{wp}=13.55%, R_p=10.70%, χ^2=1.580

Table S2 Atomic parameters of pure $Zr(HPO_4)_2 \cdot H_2O$

Atom	Wyck.	Site	S.O.F.	x/a	y/b	z/c
Zr1	4e	1	1	0.24181	0.24483	0.49857
P1	4e	1	1	0.35962	0.7426	0.38829
P2	4e	1	1	-0.1075	0.17011	0.42412
O1	4e	1	1	0.55231	0.63097	0.46964
O2	4e	1	1	0.34522	0.53595	0.37530
O3	4e	1	1	0.26976	0.93807	0.39359
O4	4e	1	1	0.28556	1.95303	0.38757
O5	4e	1	1	-0.15995	0.50362	0.39151
O6	4e	1	1	-0.18627	0.01178	0.44514
O7	4e	1	1	-0.15528	0.22693	0.29616
O8	4e	1	1	0.03263	0.40281	0.39642
O9	4e	1	1	0.03568	0.70240	0.26542
H1	4e	1	1	0.27194	-0.83556	0.16228
H2	4e	1	1	1.32656	6.78193	0.52875
H3	4e	1	1	-0.11281	2.09937	0.31864
H4	4e	1	1	0.98534	3.98886	0.64357

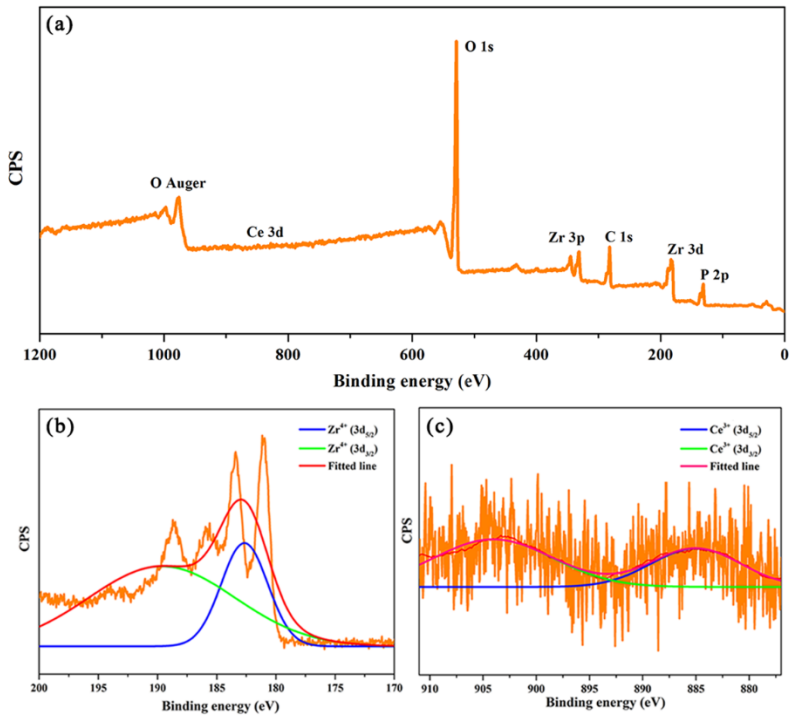

Figure. S2 (a) The full XPS spectrum of ZCG nanocomposites. (b) The fine XPS spectra of Zr^{4+}. (b) The fine XPS spectra of Ce^{3+}.

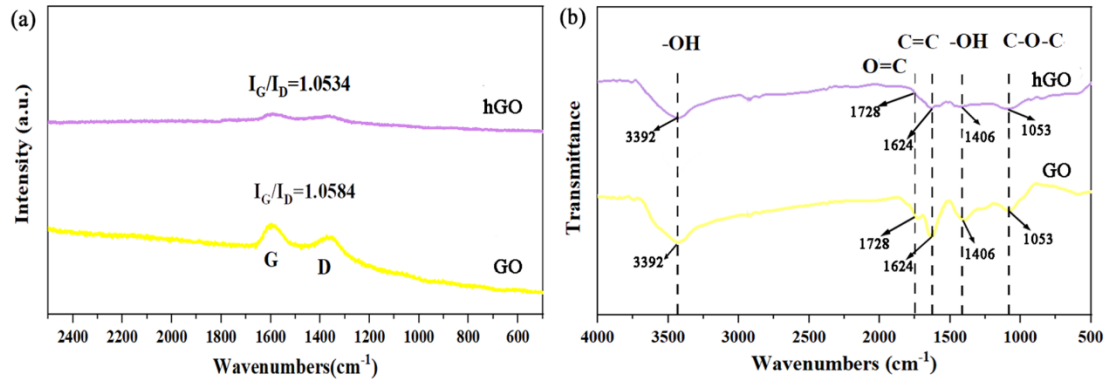

Figure. S3 The Raman test(a) and Infrared analysis(b) of hGO and GO.

Table S3 Micro calorimetry test data of Fig. 4(a)

Samples	PHRR(W/g)	Tp(℃)	HRC(J/g-K)	THR(kJ/g)
0.00 CeO_2	216.8	353.1	2186.1	22.6
0.05 CeO_2	154.0	355.1	1838.7	21.3
0.10 CeO_2	149.6	361.5	1121.9	20.2
0.15 CeO_2	148.1	373.8	1060.1	19.7
0.20 CeO_2	160.5	368.6	1951.3	20.0

Table S4 Micro calorimetry test data of Fig. 4(b)

Samples	pHRR(W/g)	Tp(℃)	HRC(J/g-K)	THR(kJ/g)
Pure PVA	216.8	353.1	2186.1	22.6
PVA/α-ZrP	172.5	373.9	1356.6	19.3
PVA/α-ZrP /CPO	145.5	374.2	518.5	18.9
PVA/ZCG	137.4	363.4	1563.9	17.94

Table S5 Micro calorimetry test data of Fig. 4(c)

Samples	pHRR(W/g)	Tp(℃)	HRC(J/g-K)	THR(kJ/g)
Pure PVA	216.8	353.1	2186.1	22.6
PVA/APP	134.1	442.	1144.6	21.1
PVA/APP/ZCG	115.2	461.3	1351.8	17.6

Table S6 The data of T-50%, Rmax, and Tmax about PVA and its flame-retardant composites in TGA/DTG

Samples	T - 50% (°C)	Rmax (%)	Tmax (°C)
Pure PVA	280.2	0.99	262.5
PVA/APP	287.1	0.86	276.1
PVA/APP/α-ZrP	290.3	0.79	268.2
PVA/APP/α-ZrP /CPO	294.1	0.81	259.5
PVA/APP/ZCG	404.9	0.76	255.6

Note. $T_{-50\%}$ was the temperature at which weight is reduced by 50%. R_{max} was the absolute value of the maximum weight loss rate. T_{max} was the maximum weight loss rate corresponding temperature of the composites.

Table S7 The elongation at break and tensile strength of PVA matrix with ZCG and APP.

Samples	Tensile Strength(MPa)	Elongation at break(%)
PVA	91.1	5.1
PVA/APP	57.9	4
PVA/ZCG	87.7	4.2
PVA/APP/ZCG	80.3	3.8

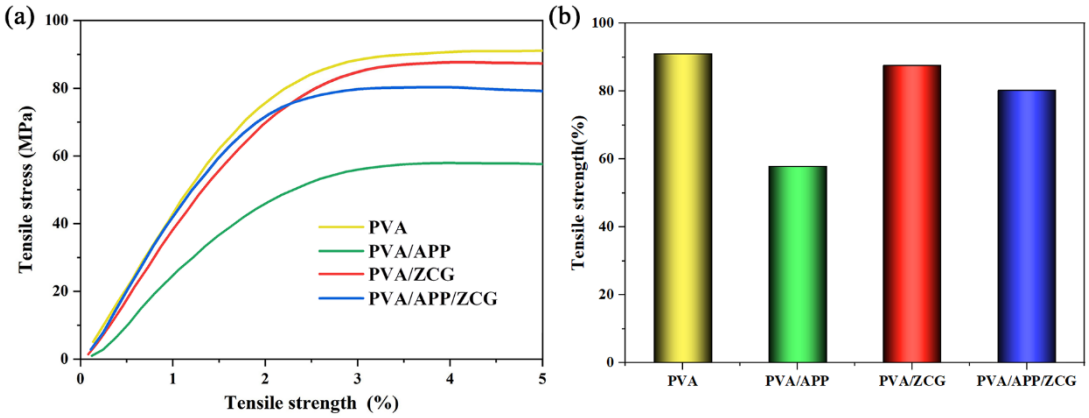

Figure. S4 (a) The stress-strain diagrams of PVA and its composites. (b) The tensile strength value of PVA and its composites.

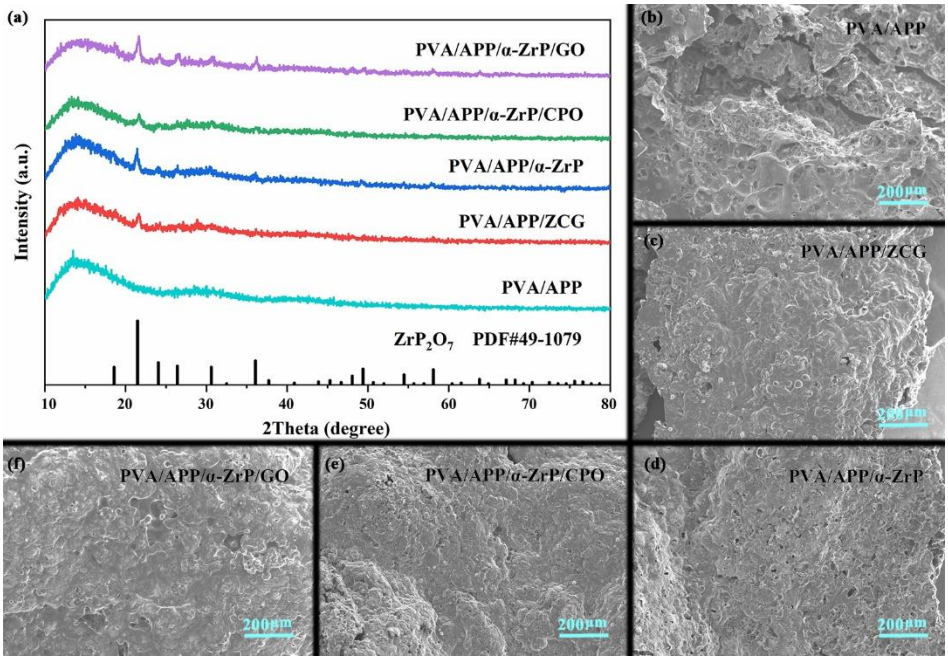

Figure S5 The XRD patterns(a) and SEM images(b-f) of char residues of PVA/APP/ZCG samples.