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Supplementary Information

The enhanced bandgap and birefringence of rare-earth phosphates XPO_4(X=Sc, Y, La, Lu) : A first-principles investigation

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Table S1 $ScPO_4$ VASP-POSCAR file information

Generated by cif2cell 1.2.10 from ICSD reference: 74483. : Failed to get author information, Powder Diffraction 8, 164-167 (1993).

6.578700000000000

1.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	1.000000000000000	0.000000000000000
0.500000000000000	0.500000000000000	0.440535364129691

Sc P O

2 2 8

Direct

0.375000000000000	0.125000000000000	0.250000000000000
0.625000000000000	0.875000000000000	0.750000000000000
0.875000000000000	0.625000000000000	0.250000000000000
0.125000000000000	0.375000000000000	0.750000000000000
0.708400000000000	0.639500000000000	0.583200000000000
0.291600000000000	0.722700000000000	0.416800000000000

0.139500000000000	0.208400000000000	0.083200000000000
0.291600000000000	0.360500000000000	0.416800000000000
0.777300000000000	0.208400000000000	0.083200000000000
0.708400000000000	0.277300000000000	0.583200000000000
0.860500000000000	0.791600000000000	0.916800000000000
0.222700000000000	0.791600000000000	0.916800000000000

Table S2 YPO_4 VASP-POSCAR file information

Generated by cif2cell 1.2.10 from ICSD reference: 79754. Y (P O4) : Failed to get author information, American Mineralogist 80, 21-26 (1995).

6.894700000000000

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Y P O

2 2 8

Direct

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0.125000000000000	0.375000000000000	0.750000000000000
0.625000000000000	0.875000000000000	0.750000000000000
0.375000000000000	0.125000000000000	0.250000000000000
0.784200000000000	0.859500000000000	0.431600000000000
0.215800000000000	0.791100000000000	0.568400000000000
0.359500000000000	0.284200000000000	0.931600000000000
0.215800000000000	0.140500000000000	0.568400000000000
0.708900000000000	0.284200000000000	0.931600000000000
0.784200000000000	0.208900000000000	0.431600000000000
0.640500000000000	0.715800000000000	0.068400000000000
0.291100000000000	0.715800000000000	0.068400000000000

Table S3 $LaPO_4$ VASP-POSCAR file information

Generated by cif2cell 1.2.10 from ICSD reference: 92155. : Failed to get author information, Revista Boliviana de Quimica 17, 22-27 (2000).

6.841300000000000

1.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	1.034598687383977	0.000000000000000
-0.219443313326914	0.000000000000000	0.926720992792641

P O La

4 16 4

Direct

0.299700000000000	0.149900000000000	0.656100000000000
0.700300000000000	0.850100000000000	0.343900000000000
0.200300000000000	0.649900000000000	0.843900000000000

0.799700000000000	0.350100000000000	0.156100000000000
0.241700000000000	0.044500000000000	0.404600000000000
0.758300000000000	0.955500000000000	0.595400000000000
0.258300000000000	0.544500000000000	0.095400000000000
0.741700000000000	0.455500000000000	0.904600000000000
0.338800000000000	0.356200000000000	0.473100000000000
0.661200000000000	0.643800000000000	0.526900000000000
0.161200000000000	0.856200000000000	0.026900000000000
0.838800000000000	0.143800000000000	0.973100000000000
0.503000000000000	0.092000000000000	0.729700000000000
0.497000000000000	0.908000000000000	0.270300000000000
0.997000000000000	0.592000000000000	0.770300000000000
0.003000000000000	0.408000000000000	0.229700000000000
0.095300000000000	0.215400000000000	0.680100000000000
0.904700000000000	0.784600000000000	0.319900000000000
0.404700000000000	0.715400000000000	0.819900000000000
0.595300000000000	0.284600000000000	0.180100000000000
0.279700000000000	0.164100000000000	0.088300000000000
0.720300000000000	0.835900000000000	0.911700000000000
0.220300000000000	0.664100000000000	0.411700000000000
0.779700000000000	0.335900000000000	0.588300000000000

Table S4 $LuPO_4$ VASP-POSCAR file information

Generated by cif2cell 1.2.10 from ICSD reference: 162336. : Failed to get author information, American Mineralogist 94, 98-104 (2009).

6.789500000000000

1.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	1.000000000000000	0.000000000000000
0.500000000000000	0.500000000000000	0.438618454967229

P Lu O

2 2 8

Direct

0.625000000000000	0.875000000000000	0.750000000000000
0.375000000000000	0.125000000000000	0.250000000000000
0.875000000000000	0.625000000000000	0.250000000000000
0.125000000000000	0.375000000000000	0.750000000000000
0.783700000000000	0.211400000000000	0.432600000000000
0.216300000000000	0.144000000000000	0.567400000000000
0.711400000000000	0.283700000000000	0.932600000000000
0.216300000000000	0.788600000000000	0.567400000000000
0.356000000000000	0.283700000000000	0.932600000000000
0.783700000000000	0.856000000000000	0.432600000000000
0.288600000000000	0.716300000000000	0.067400000000000
0.644000000000000	0.716300000000000	0.067400000000000

Table S5 Space Groups, Birefringence at 1064 nm obtained with VASP code

Crystal	Space group	1064nm				515nm			
		n_e	n_o		△n	n_e	n_o		△n
$ScPO_4$	I41/AMD	1.9458	2.0738		0.1280	1.9433	2.0675		0.1242
YPO_4	I41/AMD	1.8241	1.9170		0.0929	1.8139	1.8875		0.0836
$LuPO_4$	I41/AMD	1.8143	1.9037		0.0894	1.8374	1.9266		0.0892
Crystal	**Space group**	n_x	n_y	n_z	△n	n_x	n_y	n_z	△n
$LaPO_4$	$P12_1/a1$	1.9185	1.9078	1.9592	0.0407	1.9517	1.9452	2.0003	0.0486

Table S6 Dielectric constants of $ScPO_4$

Crystal	Optical Permittivity(f→infinity)			DC Permittivity(f=0)		
$ScPO_4$	3.39435	0.00000	0.00000	11.17167	0.00000	0.00000
	0.00000	3.39435	0.00000	0.00000	11.17167	0.00000
	0.00000	0.00000	4.26711	0.00000	0.00000	14.48357

Table S7 Dielectric constants of YPO_4

Crystal	Optical Permittivity(f→infinity)			DC Permittivity(f=0)		
YPO_4	3.00279	0.00000	0.00000	6.95848	0.00000	0.00000
	0.00000	3.00279	0.00000	0.00000	6.95848	0.00000
	0.00000	0.00000	3.52143	0.00000	0.00000	8.22851

Table S8 Dielectric constants of $LaPO_4$

Crystal	Optical Permittivity(f→infinity)			DC Permittivity(f=0)		
$LaPO_4$	3.17173	0.00000	0.00645	7.42583	0.00000	0.42787
	0.00000	3.17088	0.00000	0.00000	6.86640	0.00000
	0.00000	0.00000	3.54443	0.42787	0.00000	9.44489

Table S9 Dielectric constants of $LuPO_4$

Crystal	Optical Permittivity(f→infinity)			DC Permittivity(f=0)		
$LuPO_4$	3.26853	0.00000	0.00000	10.92020	0.00000	0.00000
	0.00000	3.26853	0.00000	0.00000	10.92020	0.00000
	0.00000	0.00000	3.73368	0.00000	0.00000	11.37405

Table S10 Distortion index of PO_4 polyhedra in XPO_4 (X = Sc, Y, La, Lu) compounds.

Crystal	Group	Distortion index
$LaPO_4$	PO_4	0.00564
$LuPO_4$	PO_4	0
YPO_4	PO_4	0

$ScPO_4$	PO_4	0

Table S11 Born effective charge of $ScPO_4$

atom	Born effective charges		
O(1)	-1.02418	-0.00000	-0.00000
	-0.00000	-2.47191	-0.40882
	-0.00000	-0.56159	-2.34064
O(2)	-1.02418	0.00000	-0.00000
	0.00000	-2.47191	0.40882
	-0.00000	0.56159	-2.34064
O(3)	-2.47191	0.00000	0.40882
	0.00000	-1.02418	0.00000
	0.56159	0.00000	-2.34064
O(4)	-2.47191	0.00000	-0.40882
	0.00000	-1.02418	0.00000
	-0.56159	0.00000	-2.34064
O(5)	-1.02418	0.00000	-0.00000
	0.00000	-2.47191	0.40882
	-0.00000	0.56159	-2.34064
O(6)	-1.02418	-0.00000	-0.00000
	-0.00000	-2.47191	-0.40882
	-0.00000	-0.56159	-2.34064
O(7)	-2.47191	0.00000	0.40882
	0.00000	-1.02418	0.00000
	0.56159	0.00000	-2.34064
O(8)	-2.47191	0.00000	-0.40882
	0.00000	-1.02418	0.00000
	-0.56159	0.00000	-2.34064
P(1)	3.21024	-0.00000	0.00000
	-0.00000	3.21024	-0.00000

	0.00000	-0.00000	4.86689
P(2)	3.21024	-0.00000	0.00000
	-0.00000	3.21024	-0.00000
	0.00000	-0.00000	4.86689
Sc(1)	3.78195	-0.00000	0.00000
	-0.00000	3.78195	-0.00000
	0.00000	-0.00000	4.49568
Sc(2)	3.78195	-0.00000	0.00000
	-0.00000	3.78195	-0.00000
	0.00000	-0.00000	4.49568

Table S12 Born effective charge of YPO_4

atom	Born effective charges		
O(1)	-1.03565	-0.00000	0.00000
	-0.00000	-2.41896	-0.47623
	0.00000	-0.56411	-2.16757
O(2)	-1.03565	-0.00000	0.00000
	-0.00000	-2.41896	0.47623
	0.00000	0.56411	-2.16757
O(3)	-2.41896	-0.00000	0.47623
	-0.00000	-1.03565	-0.00000
	0.56411	-0.00000	-2.16757
O(4)	-2.41896	-0.00000	-0.47623
	-0.00000	-1.03565	-0.00000
	-0.56411	-0.00000	-2.16757
O(5)	-1.03565	-0.00000	0.00000
	-0.00000	-2.41896	0.47623
	0.00000	0.56411	-2.16757
O(6)	-1.03565	-0.00000	0.00000
	-0.00000	-2.41896	-0.47623

	0.00000	-0.56411	-2.16757
O(7)	-2.41896	-0.00000	0.47623
	-0.00000	-1.03565	-0.00000
	0.56411	-0.00000	-2.16757
O(8)	-2.41896	-0.00000	-0.47623
	-0.00000	-1.03565	-0.00000
	-0.56411	-0.00000	-2.16757
P(1)	3.26594	0.00000	-0.00000
	0.00000	3.26594	0.00000
	-0.00000	0.00000	4.35488
P(2)	3.26594	0.00000	-0.00000
	0.00000	3.26594	0.00000
	-0.00000	0.00000	4.35488
Y(1)	3.64329	0.00000	-0.00000
	0.00000	3.64329	0.00000
	-0.00000	0.00000	4.31540
Y(2)	3.64329	0.00000	-0.00000
	0.00000	3.64329	0.00000
	-0.00000	0.00000	4.31540

Table S13 Born effective charge of $LaPO_4$

atom	Born effective charges		
O(1)	-1.12346	-0.18380	-0.08971
	-0.27592	-2.29177	-0.35070
	-0.08956	-0.41761	-2.25113
O(2)	-1.62144	-0.13483	0.11545
	-0.09193	-2.07869	0.43129
	0.14245	0.44811	-1.80163
O(3)	-1.98530	0.50891	-0.28329
	0.40730	-1.49505	0.19482

	-0.38376	0.21355	-2.18926
O(4)	-2.18852	0.49337	0.19499
	0.44983	-1.24542	-0.03884
	0.30624	-0.08077	-2.10515
O(5)	-1.12346	0.18380	-0.08971
	0.27592	-2.29177	0.35070
	-0.08956	0.41761	-2.25113
O(6)	-1.62144	0.13483	0.11545
	0.09193	-2.07869	-0.34129
	0.14245	-0.44811	-1.80163
O(7)	-1.98530	-0.50891	-0.28329
	-0.40730	-1.49505	-0.19482
	-0.38376	-0.21355	-2.18926
O(8)	-2.18852	-0.49337	0.19499
	-0.44983	-1.24542	0.03884
	0.30624	0.08077	-2.10515
O(9)	-1.12346	-0.18380	-0.08971
	-0.27592	-2.29177	-0.35070
	-0.08956	-0.41761	-2.25113
O(10)	-1.62144	-0.13483	0.11545
	-0.09193	-2.07869	0.34129
	0.14245	0.44811	-1.80163
O(11)	-1.98530	0.50891	-0.28329
	0.40730	-1.49505	0.19482
	-0.38376	0.21355	-2.18926
O(12)	-2.18852	0.49337	0.19499
	0.44983	-1.24542	-0.03884
	0.30624	-0.08077	-2.10515
O(13)	-1.12346	0.18380	-0.08971

	0.27592	-2.29177	0.35070
	-0.08956	0.41761	-2.25113
O(14)	-1.62144	0.13483	0.11545
	0.09193	-2.07869	-0.34129
	0.14245	-0.44811	-1.80163
O(15)	-1.98530	-0.50891	-0.28329
	-0.40730	-1.49505	-0.19482
	-0.38376	-0.21355	-2.18926
O(16)	-2.18852	-0.49337	0.19499
	-0.44983	-1.24542	0.03884
	0.30624	0.08077	-2.10515
P(1)	3.17320	-0.09824	0.03049
	-0.07234	3.26603	0.01974
	-0.02418	-0.02943	4.02577
P(2)	3.17320	0.09824	0.03049
	0.07234	3.26603	-0.01974
	-0.02418	0.02934	4.02577
P(3)	3.17320	-0.09824	0.03049
	-0.07234	3.26603	0.01974
	-0.02418	-0.02934	4.02577
P(4)	3.17320	0.09824	0.03049
	0.07234	3.26603	-0.01974
	-0.02418	-0.02934	4.02577
La(1)	3.74552	-0.11704	0.03207
	-0.19070	3.84491	-0.16423
	0.04881	-0.07023	4.32141
La(2)	3.74552	0.11704	0.03207
	0.19070	3.84491	0.16423
	0.04881	-0.07023	4.32141

La(3)	3.74552	-0.11704	0.03207
	-0.19070	3.84491	-0.16423
	0.04881	-0.07023	4.32141
La(4)	3.74552	0.11704	0.03207
	0.19070	3.84491	0.16423
	0.04881	-0.07023	4.32141

Table S14 Born effective charge of $LuPO_4$

atom	Born effective charges		
O(1)	-0.99078	0.00000	-0.00000
	-0.00000	-2.56360	0.52166
	-0.00000	0.58362	-2.28904
O(2)	-0.99078	0.00000	-0.00000
	0.00000	-2.56360	-0.52166
	-0.00000	-0.58362	-2.28904
O(3)	-2.56360	0.00000	-0.52166
	0.00000	-0.99078	-0.0000
	-0.58362	-0.00000	-2.28904
O(4)	-2.56360	0.00000	0.52166
	0.00000	-0.99078	-0.0000
	0.58362	-0.00000	-2.28904
O(5)	-0.99078	0.00000	-0.00000
	0.00000	-2.56360	-0.52166
	-0.00000	-0.58362	-2.28904
O(6)	-0.99078	0.00000	-0.00000
	0.00000	-2.56360	0.52166
	-0.00000	0.58362	-2.28904
O(7)	-2.56360	0.00000	-0.52166
	0.00000	-0.99078	-0.0000

	-0.58362	-0.00000	-2.28904
O(8)	-2.56360	0.00000	0.52166
	0.00000	-0.99078	-0.0000
	0.58362	-0.00000	-2.28904
P(1)	3.27451	-0.00000	0.00000
	-0.00000	3.27451	0.00000
	0.00000	0.00000	4.74688
P(2)	3.27451	-0.00000	0.00000
	-0.00000	3.27451	0.00000
	0.00000	0.00000	4.74688
Lu(1)	3.83425	-0.00000	0.00000
	-0.00000	3.83425	0.00000
	0.00000	0.00000	4.40929
Lu(2)	3.83425	-0.00000	0.00000
	-0.00000	3.83425	0.00000
	0.00000	0.00000	4.40929

Table S15 Distortion index of XO_8 polyhedra in XPO_4 (X = Sc, Y, La, Lu) compounds.

Crystal	Group	Distortion index
$ScPO_4$	ScO_8	0.02652
YPO_4	YO_8	0.01549
$LaPO_4$	LaO_8	0.03421
$LuPO_4$	LuO_8	0.01784

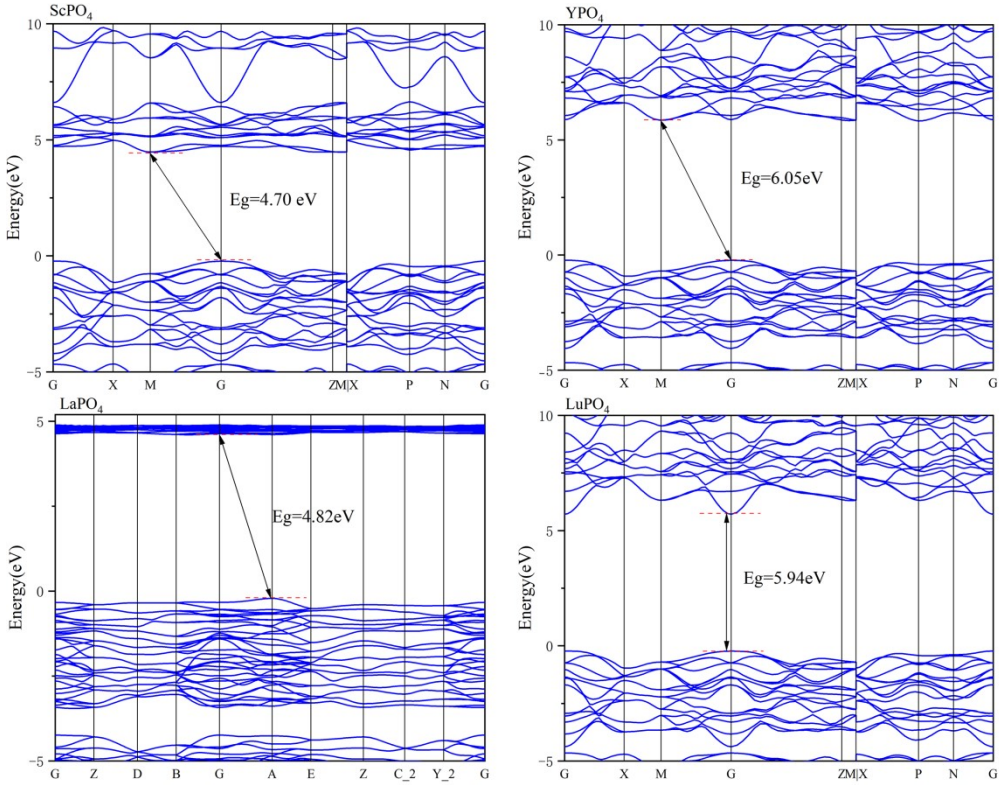

Fig S1 Band structures of XPO_4(X=Sc, Y, La, Lu) obtained by GGA/PBE functional implemented in VASP code.

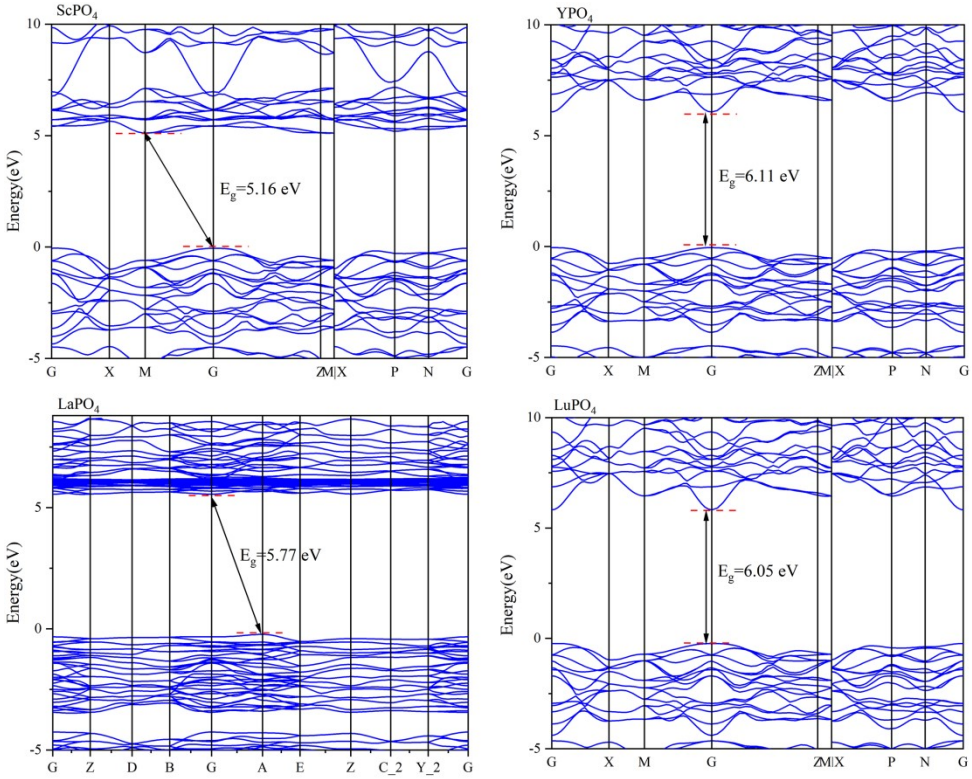

Fig S2 Band structures of XPO_4(X=Sc, Y, La, Lu) obtained by GGA+U functional implemented in VASP code.

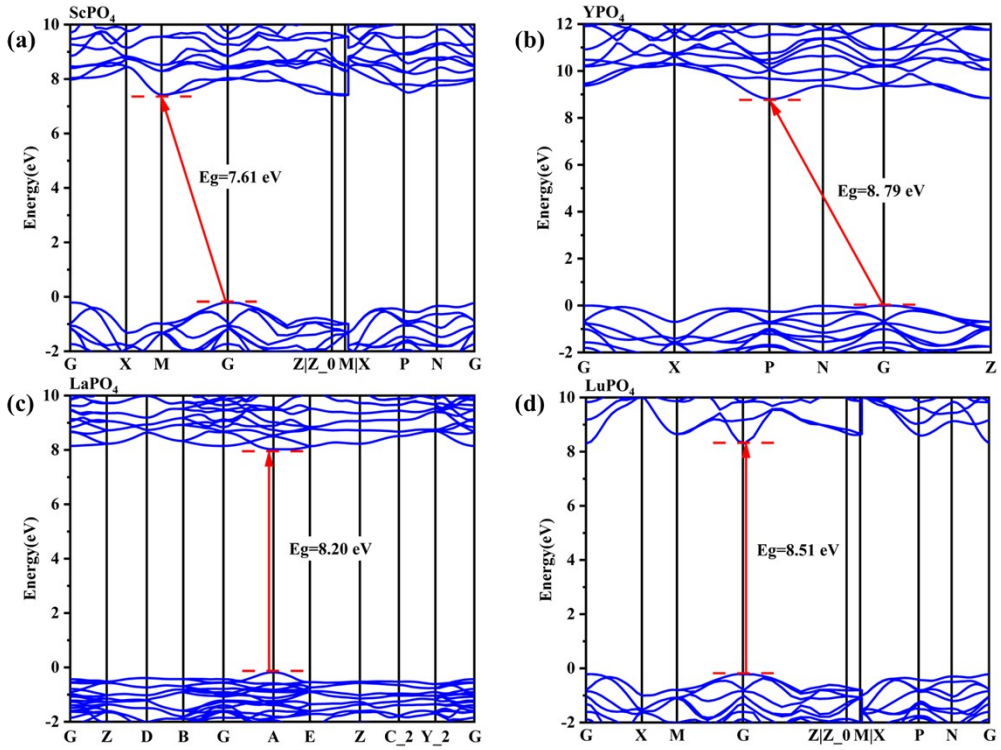

Fig S3 The band structures of XPO_4 (X=Sc, Y, La, Lu) implemented in the PWMAT code using the HSE06 functional, where (a) is $ScPO_4$, (b) is YPO_4, (c) is $LaPO_4$, and (d) is $LuPO_4$.

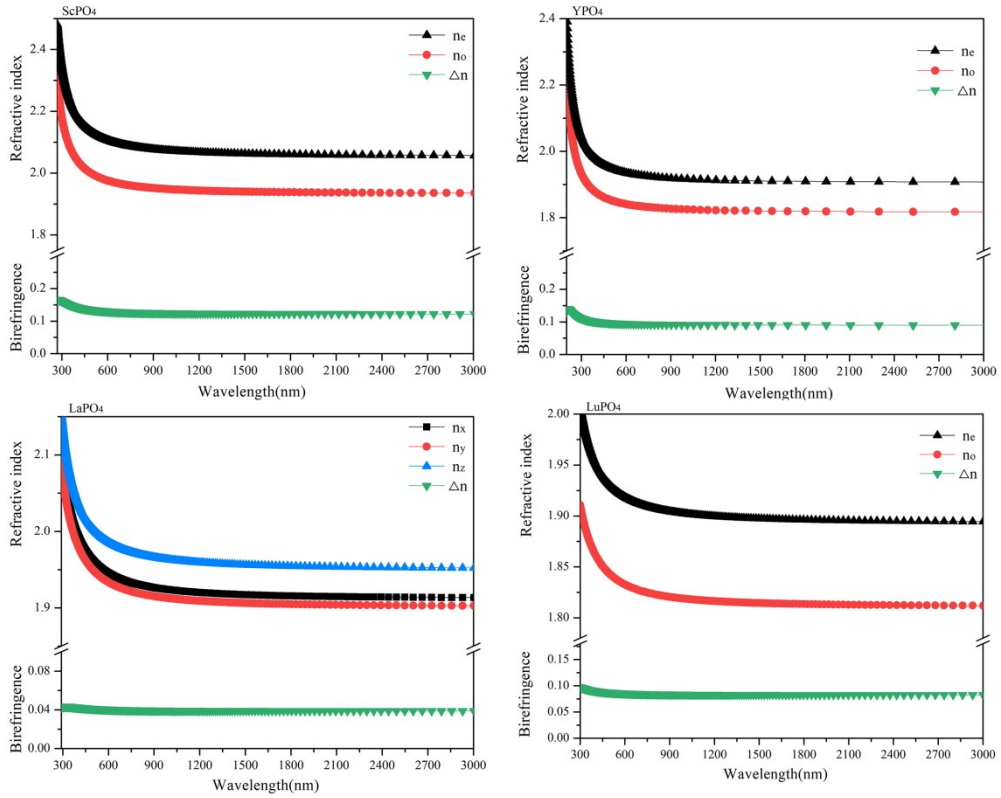

Fig S4 The the refractive indices and birefringence obtained by GGA/PBE functional concerning Hubbard picture implemented in VASP code.

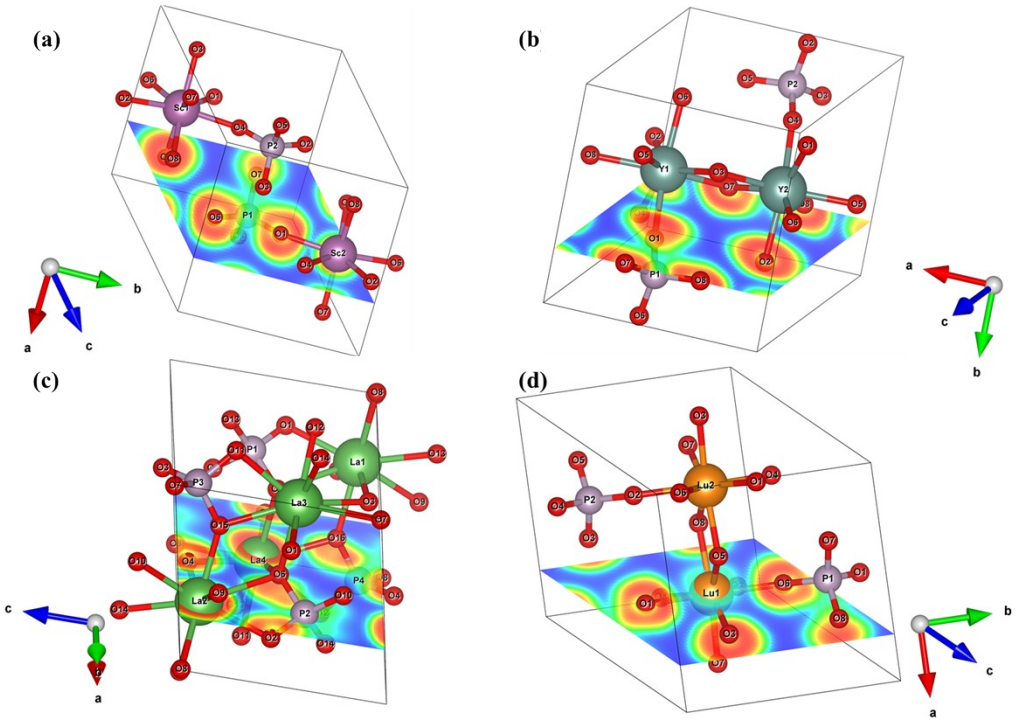

Fig S5 Electron Localization Function (ELF) of XPO_4 (X = Sc, Y, La, Lu) obtained by VASP code, where (a) is $ScPO_4$, (b) is YPO_4, (c) is $LaPO_4$, (d) is $LuPO_4$.

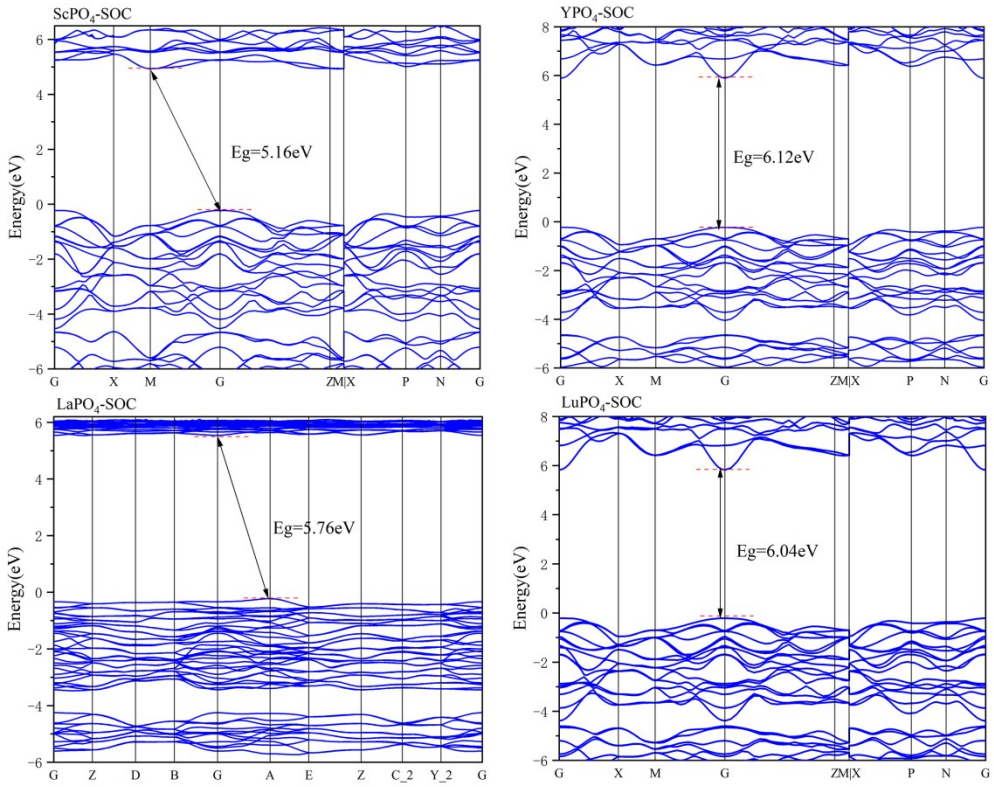

Fig S6 The band structures of XPO_4 (X=Sc, Y, La, Lu) considering SOC were calculated using the GGA+PBE functional in the VASP code.