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Supporting Information

Experimental and Theoretical Studies on the Linear and Nonlinear Optical Properties of Lead Phosphate Crystal $LiPbPO_4$

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Table S1. Atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $LiPbPO_4$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atoms	Wyck.	*x*	*y*	*z*	*U*(eq)
Pb(1)	4*a*	3257(10)	4465(10)	885(10)	12(10)
Pb(2)	4*a*	4727(10)	2290(10)	729(20)	15(10)
P(1)	4*a*	2670(40)	716(20)	379(10)	8(10)
P(2)	4*a*	2877(50)	3204(20)	5339(90)	8(10)
Li(1)	4*a*	4910(30)	592(12)	-4610(60)	11(50)
Li(2)	4*a*	1800(30)	1489(13)	-4640(60)	12(60)
O(1)	4*a*	2815(13)	738(60)	3460(20)	9(20)
O(2)	4*a*	2479(13)	1478(60)	-790(20)	12(20)
O(3)	4*a*	1367(13)	3645(60)	4540(20)	17(30)
O(4)	4*a*	3087(14)	3180(70)	8420(20)	16(30)
O(5)	4*a*	1082(13)	275(60)	-440(20)	11(20)
O(6)	4*a*	4160(14)	342(60)	-930(20)	11(20)
O(7)	4*a*	4436(13)	3531(60)	3990(20)	13(20)
O(8)	4*a*	2695(14)	2445(60)	4200(20)	14(20)

Table S2. Selected bond lengths (Å) and angles (°) for $LiPbPO_4$.

Pb(1)-O(5)#1	2.410(10)	O(4)#3-Pb(1)-O(6)#11	85.753(30)
Pb(1)-O(5)#2	2.431(11)	O(1)#13-Pb(1)-O(3)	124.969(31)
Pb(1)-O(7)	2.513(12)	O(1)#13-Pb(1)-O(6)#2	64.076(31)
Pb(1)-O(4)#3	2.698(12)	O(1)#13-Pb(1)-O(6)#11	60.211(28)
Pb(1)-O(1) #2	2.8018(11)	O(3)-Pb(1)-O(6)#2	66.954(29)
Pb(1)-O(3)	2.8183(10)	O(3)-Pb(1)-O(6)#11	73.153(28)
Pb(1)-O(6)#2	2.9917(11)	O6#2-Pb(1)-O(6)#11	57.272(29)
Pb(1)-O(6)#11	3.4289(12)	O(8)-Pb(2)-O(7)	55.486(33)
Pb(2)-O(8)	2.389(11)	O(8)-Pb(2)-O(3)#1	84.971(32)
Pb(2)-O(4)#3	2.411(12)	O(8)-Pb(2)-O(8)#1	96.214(33)
Pb(2)-O(2)	2.474(11)	O(8)-Pb(2)-O(4)#6	155.03(33)
Pb(2)-O(7)	2.8389(11)	O(8)-Pb(2)-O(2)#1	122.684(32)
Pb(2)-O(3)#1	2.8921(11)	O(4)#3-Pb(2)-O(7)	70.260(37)
Pb(2)-O(8)#1	2.9821(11)	O(4)#3-Pb(2)-O(3)#1	167.472(34)
Pb(2)-O(4) #6	3.0594(12)	O(4)#3-Pb(2)-O(8)#1	126.578(33)
Pb(2)-O(2)#1	3.2795(11)	O(4)#3-Pb(2)-O(4)#6	120.063(35)
P(1)-O(6)	1.529(11)	O(4)#3-Pb(2)-O(2)#1	76.918(34)
P(1)-O(1)	1.534(11)	O(2)-Pb(2)-O(7)	127.935(33)
P(1)-O(2)	1.546(12)	O(2)-Pb(2)-O(3)#1	99.278(32)
P(1)-O(5)	1.571(11)	O(2)-Pb(2)-O(8)#1	149.383(32)
P(2)-O(3)	1.519(11)	O(2)-Pb(2)-O(4)#6	110.660(32)
P(2)-O(8)	1.536(12)	O(2)-Pb(2)-O(2)#1	148.374(31)
P(2)-O(4)	1.542(11)	O(7)-Pb(2)-O(3)#1	99.082(31)
P(2)-O(7)	1.546(11)	O(7)-Pb(2)-O(8)#1	66.428(29)
Li(1)-O(3)#6	1.89(20)	O(7)-Pb(2)-O(4)#6	121.372(30)
Li(1)-O(1)#3	1.95(30)	O(7)-Pb(2)-O(2)#1	67.200(29)
Li(1)-O(6)	1.98(30)	O(3)#1-Pb(2)-O(8)#1	50.107(29)
Li(1)-O(6)#7	2.01(30)	O(3)#1-Pb(2)-O(4)#6	70.766(30)
Li(2)-O(1)#3	1.88(30)	O(3)#1-Pb(2)-O(2)#1	105.540(28)
Li(2)-O(2)	1.99(30)	O(8)#1-Pb(2)-O(4)#6	63.886(30)
Li(2)-O(8)#3	2.01(30)	O(8)#1-Pb(2)-O(2)#1	58.520(28)
Li(2)-O(7)#10	2.01(30)	O4#6-Pb(2)-O(2)#1	61.402(28)
O(5)#1-Pb(1)-O(5)#2	82.7(30)	O(8)-Pb(2)-O(4)#3	83.4(40)
O(5)#1-Pb(1)-O(7)	87.3(30)	O(8)-Pb(2)-O(2)	78.2(40)
O(7)-Pb(1)-O(4)#3	71.2(30)	O(4)#3-Pb(2)-O(2)	83.1(40)
O(5)#2-Pb(1)-O(7)	83.7(40)	O(6)-P(1)-O(1)	112.1(60)
O(5)#1-Pb(1)-O(4)#3	96.0(40)	O(6)-P(1)-O(2)	109.9(60)
O(5)#2-Pb(1)-O(4)#3	154.9(40)	O(1)-P(1)-O(2)	110.9(60)
O(5)#1-Pb(1)-O(1)#13	90.024(34)	O(6)-P(1)-O(5)	106.6(60)
O(5)#1-Pb(1)-O(3)	142.343(33)	O(1)-P(1)-O(5)	109.4(60)
O(5)#1-Pb(1)-O(6)#2	130.078(33)	O(2)-P(1)-O(5)	107.8(60)
O(5)#1-Pb(1)-O(6)#11	144.023(31)	O(3)-P(2)-O(8)	109.2(70)

O(5)#2-Pb(1)-O(1)#13	81.995(34)	O(3)-P(2)-O(4)	111.3(70)
O(5)#2-Pb(1)-O(3)	88.444(32)	O(8)-P(2)-O(4)	110.5(70)
O(5)#2-Pb(1)-O(6)#2	53.369(32)	O(3)-P(2)-O(7)	108.5(70)
O(5)#2-Pb(1)-O(6)#11	109.959(30)	O(8)-P(2)-O(7)	106.3(60)
O(7)-Pb(1)-O(1)#13	165.647(33)	O(4)-P(2)-O(7)	110.8(60)
O(7)-Pb1-O(3)	55.266(32)	O(3)#6-Li(1)-O(1)#3	108.5(13)
O(7)-Pb1-O(6)#2	107.485(32)	O(3)#6-Li(1)-O(6)	124.9(15)
O(7)-Pb1-O(6)#11	126.537(30)	O(1)#3-Li(1)-O(6)	103.0(11)
O(4)#3-Pb1-O(1)#13	123.035(36)	O(3)#6-Li(1)-O(6)#7	110.5(13)
O(4)#3-Pb1-O(3)	77.346(33)	O(1)#3-Li(1)-O(6)#7	106.4(12)
O(4)#3-Pb1-O(6)#2	133.981(32)	O(6)-Li(1)-O(6)#7	102.0(11)

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,-y+1/2,z	#2 -x+1/2,y+1/2,z+1/2	#3 x,y,z-1
#4 x-1/2,-y+1/2,z+1	#5 x,y,z+1	#6 x+1/2,-y+1/2,z-1
#7 -x+1,-y,z-1/2	#8 -x+1/2,y-1/2,z-1/2	#9 -x+1,-y,z+1/2
#10 x-1/2,-y+1/2,z-1	#11 x-1/2,-y+1/2,z	#12 x+1/2,-y+1/2,z+1
#13 -x+1/2,y+1/2,z-1/2		

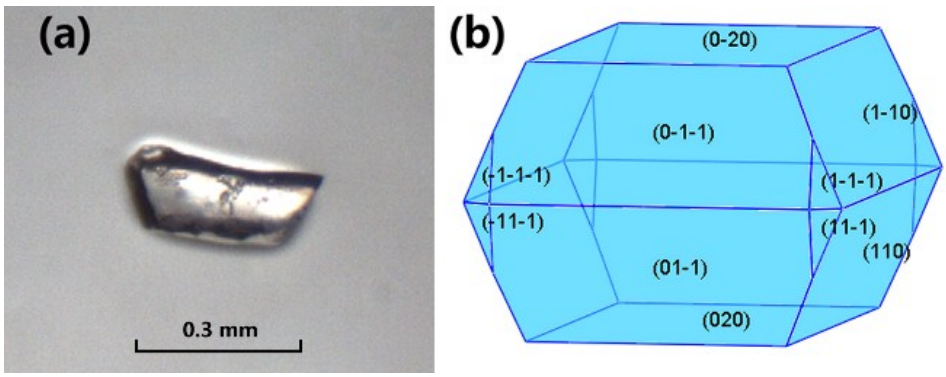

Fig. S1 (a) Photo of $LiPbPO_4$ single crystal by spontaneous crystallization; (b) Theoretical morphology of $LiPbPO_4$.

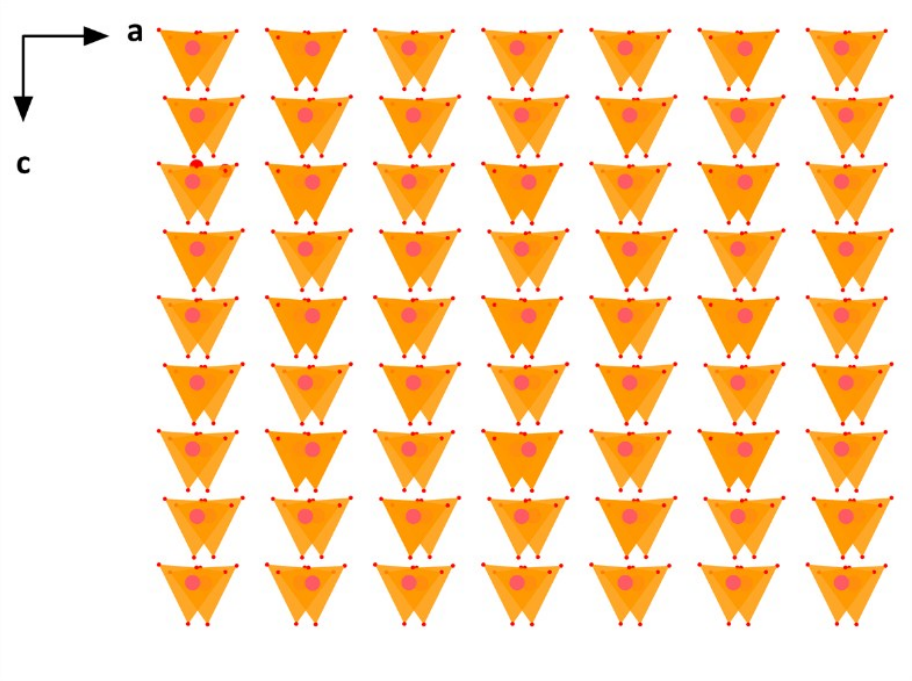

Fig. S2 Anionic groups arrangement of the PO_4 tetrahedra for $LiPbPO_4$

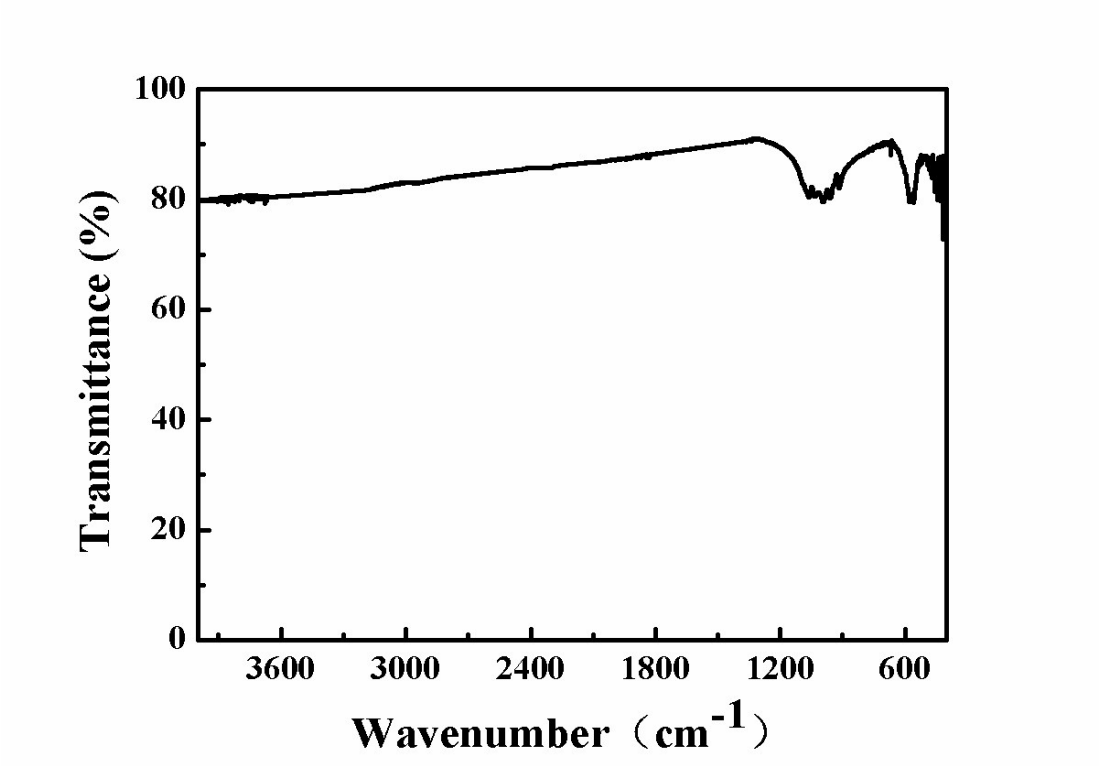

Fig. S3 The IR spectrum of as-synthesized $LiPbPO_4$.

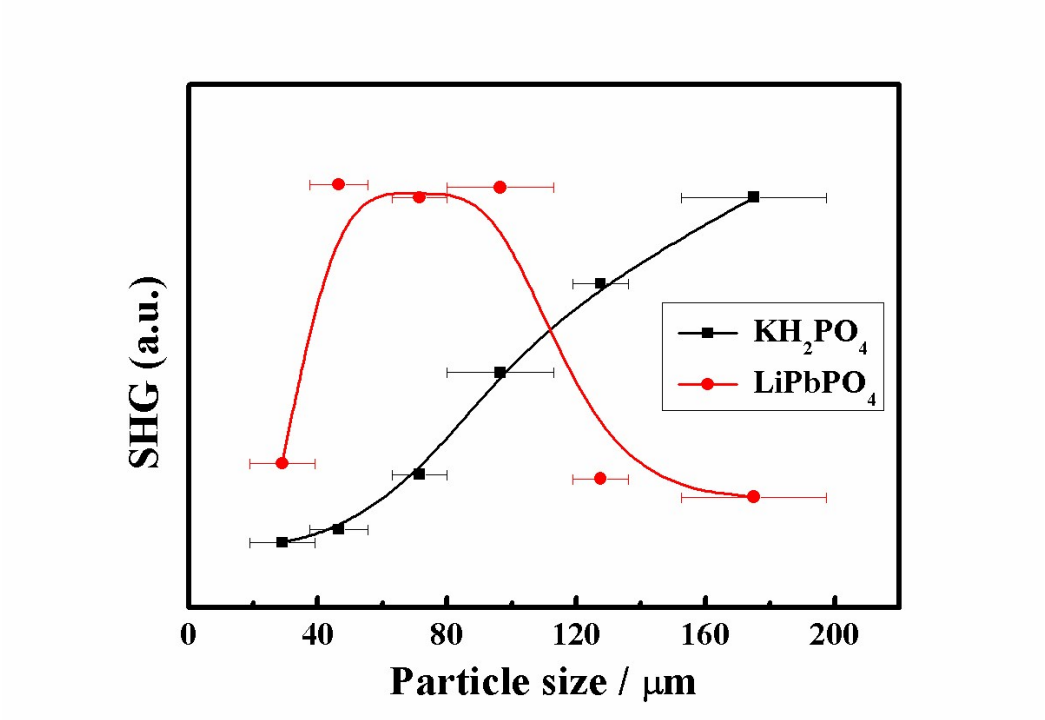

Fig. S4 SHG phase- matching curve, particle size *vs* SHG efficiency for $LiPbPO_4$. (The curve drawn is to guide the eye and is not a fit to the data.)

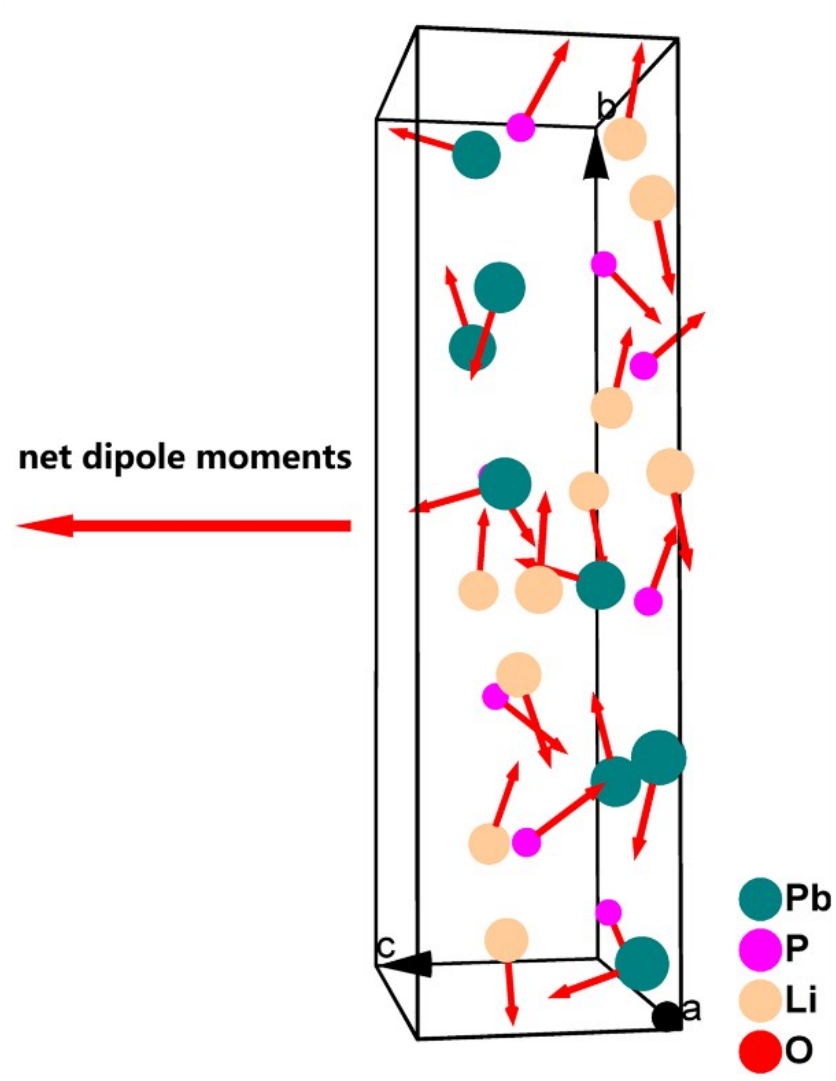

Fig. S5 The dipole moments for the PO_4 tetrahedra, the LiO_4 tetrahedra and the PbO_8 polyhedra in the unit cells of $LiPbPO_4$. The red arrows indicate the approximate direction of the dipole moments.

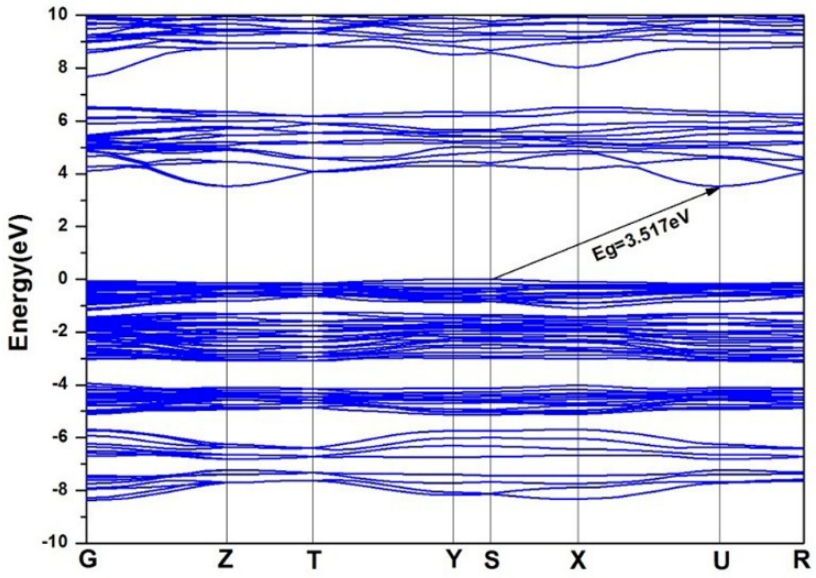

Fig. S6 The calculated band structure of $LiPbPO_4$