Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

$LiGeBO_4$: A Deep-ultraviolet Nonlinear Optical Material with Large Nonlinear Optical Response Induced by the Hand-in-hand Tetrahedra

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TableS1. Crystal data and structure refinement for $LiGeBO_4$

	$LiGeBO_4$
Formula weight	154.34
Temperature (K)	296(2)
Wavelength (Å)	0.71073
Crystal system, Space group	Tetragonal, *I*-4
Unit cell dimensions(Å)	a = 4.4273(19)
	b = 4.4273(19)
	c = 6.785(6)
Z, Volume ($Å^3$)	2
Calculated density (g/cm^3)	3.854
Absorption coefficient (mm^{-1})	11.307
F(000)	144
Theta range for data collection	5.50 to 27.38
Limiting indices	-5≤h≤3, -5≤k≤5, -8≤l≤8
Reflections collected/unique	410 / 151
Completeness to theta = 27.38	98.8 %
Data/restraints/parameters	151 / 0 / 16
Goodness-of-fit on F^2	0.522
Final R indices [I>2sigma(I)][a]	R_1 = 0.0176, wR_2 = 0.0444
R indices (all data)	R_1 = 0.0176, wR_2 = 0.0444
Largest diff. peak and hole(e. $Å^{-3}$)	0.281 and -0.554

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w F_o^4]^{1/2}$ for $F_o^2 > 2\sigma(F_o^2)$ and $w^{-1} = \sigma^2(F_o^2) + (0.0254\ P)^2 + 0.49P$ where $P = (F_o^2 + 2F_c^2)/3$.

Table S2. Atomic coordinates and equivalent isotropic displacement parameters of $LiGeBO_4$

Atom	Wyck	x/a	y/b	z/c	U[Å2]	BVS
Li1	2a	0	0	0	0.013(2)	1.04
Ge1	2b	0.5000	0.5000	0	0.0026(2)	4.33
B1	2d	0.5000	0	0.2500	0.0056(16)	3.22
O1	8g	0.3314(6)	0.2149(6)	0.1319(4)	0.0061(5)	2.15

Table S3 Selected bond distances (Å) and angles (deg.) for $LiGeBO_4$

Li1-O1	1.965(2)	B1-O1$^{\#7}$	1.451(3)
Li1-O1$^{\#4}$	1.965(2)	B1-O1$^{\#8}$	1.451(3)
Li1-O1$^{\#5}$	1.965(2)	B1-O1$^{\#9}$	1.451(3)
Li1-O1$^{\#6}$	1.965(2)	O1$^{\#1}$- Ge1- O1$^{\#2}$	105.75(9)
Ge1-O1	1.718(3)	O1$^{\#2}$-Ge1- O1$^{\#2}$	117.20(19)
Ge1-O1$^{\#1}$	1.718(3)	O1-Li1-O1$^{\#10}$	125.79(16)
Ge1-O1$^{\#2}$	1.718(3)	O1-Li1-O1$^{\#11}$	101.98(7)
Ge1-O1$^{\#3}$	1.718(3)	O1$^{\#7}$-B1-O1$^{\#9}$	112.9(2)
B1-O1	1.451(3)	O1-B1-O1$^{\#9}$	107.76(11)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, -y+1, z #2 y, -x+1, -z #3 -y+1, x, -z #4 x+1, y+1, z #5 x+1, y, z

#6 x, y+1, z #7 y+1/2, -x+1/2, -z+1/2 #8 -x+1, -y, z #9 -y+1/2, x-1/2, -z+1/2

#10 -x, -y, z #11 y, -x, -z

Figure S1. The powder XRD of $LiGeBO_4$

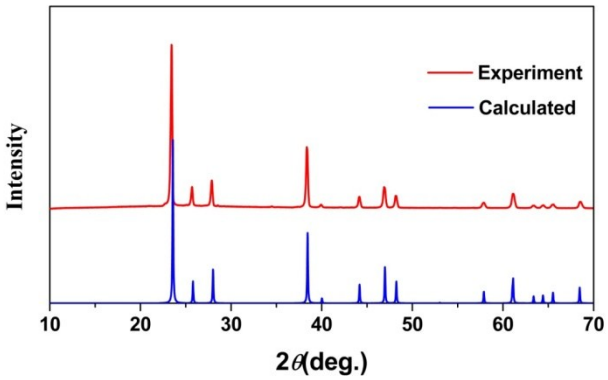

Figure S2. The bandstructure of $LiGeBO_4$

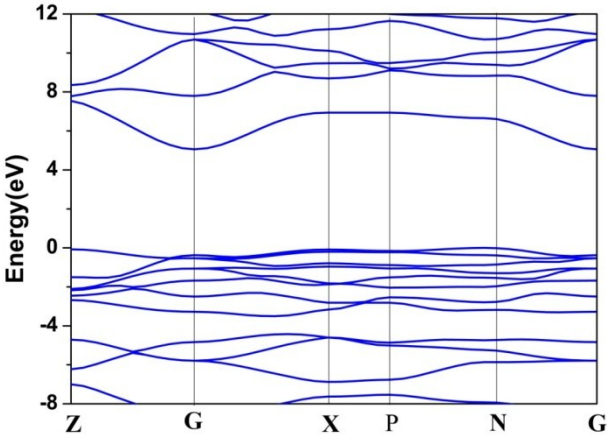

Figure S3 The TG-DSC curves of $LiGeBO_4$

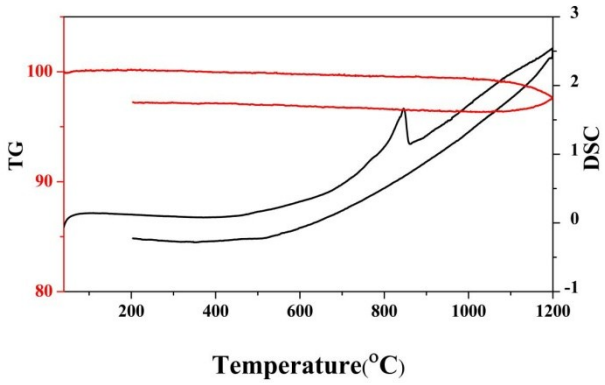

Figure S4 The IR spectrum of $LiGeBO_4$

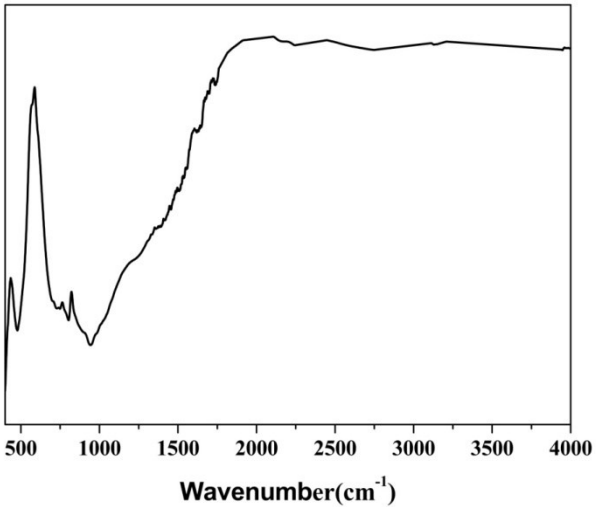

Figure S5 The UV-Vis-NIR spectrum of $LiGeBO_4$