Electronic supplementary information (ESI)

Li_2CdSiS_4, a promising IR NLO material with balanced E_g and SHG response originated from the effect of Cd with d^{10} configuration

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Supplementary Information (SI)

1. Tables and Figures

Table S1. Bond length and angles in Li_2CdSiS_4.

Li(1)-S(1)#3	2.418(7)	S(2)-Cd(1)-S(3)#3	109.36(3)
Li(1)-S(3)#1	2.42(2)	S(1)#1-Cd(1)-S(3)#3	108.31(3)
Li(1)-S(3)#9	2.444(8)	S(3)#2-Cd(1)-S(3)#3	110.66(4)
Cd(1)-S(2)	2.5174(15)	S(2)-Si(1)-S(1)	110.71(10)
Cd(1)-S(1)#1	2.5447(17)	S(2)-Si(1)-S(3)#4	108.76(7)
Cd(1)-S(3)#2	2.5555(11)	S(1)-Si(1)-S(3)#4	111.13(7)
Cd(1)-S(3)#3	2.5555(11)	S(2)-Si(1)-S(3)	108.76(7)
Si(1)-S(2)	2.113(3)	S(1)-Si(1)-S(3)	111.13(7)
Si(1)-S(1)	2.1210(17)	S(3)#4-Si(1)-S(3)	106.21(9)
Si(1)-S(3)#4	2.1301(14)	S(3)#1-Li(1)-S(3)#9	108.1(5)
Si(1)-S(3)	2.1301(14)	S(2)-Cd(1)-S(1)#1	110.84(4)
S(2)-Li(1)-S(1)#3	107.1(5)	S(2)-Cd(1)-S(3)#2	109.36(3)
S(2)-Li(1)-S(3)#1	110.6(4)	S(1)#1-Cd(1)-S(3)#2	108.31(3)
S(1)#3-Li(1)-S(3)#1	109.1(5)	S(1)#3-Li(1)-S(3)#9	115.1(5)
S(2)-Li(1)-S(3)#9	106.8(5)		

Symmetry transformations used to generate equivalent atoms:

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

Table S2. Atomic coordinates, isotropic displacement parameters and BVS for Li_2CdSiS_4.

Atoms	x	y	z	δ_{iso}	BVS
Li(1)	-2547(7)	3296(6)	8690(30)	0.022(1)	1.10
Cd(1)	0	-1435(1)	8682(1)	0.018(1)	2.10
Si(1)	0	1758(1)	3708(4)	0.011(1)	4.03
S(1)	0	-1224(2)	2712(2)	0.014(1)	2.08
S(2)	0	1948(2)	7053(2)	0.015(1)	2.21
S(3)	-2238(1)	3283(1)	2519(1)	0.014(1)	2.02

Table S3. The quantitative analysis of the chemical composition in Li_2CdSiS_4.

	Atom No.	unn. C (wt%)	norm. C (wt%)	Atom. C (at%)
Cd	48	34.48	43.7	54.67
Si	14	31.58	40.02	14.28
S	16	7.16	9.07	12.95

Table S4. Comparison of the optical properties about Li_2CdSiS_4, Li_2CdGeS_4, Li_2CdSnS_4 and $AgGaS_2$.

Formula	Space Group	Band Gap(eV)	SHG (× AGS)
$AgGaS_2$	I-*42*d	2.76	1
Li_2CdSiS_4	Pmn*2*$_1$	3.76	1
Li_2CdGeS_4	Pmn*2*$_1$	3.15	2
Li_2CdSnS_4	Pmn*2*$_1$	3.26	2.8(NPM)

Fig. S1. Crystal picture of Li_2CdSiS_4.

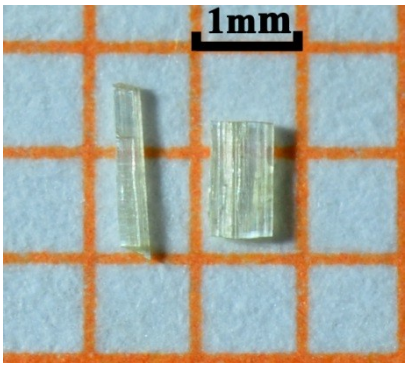

Fig. S2. Rietveld refinement XRD patterns and parameters of the powder XRD of Li_2CdSiS_4.

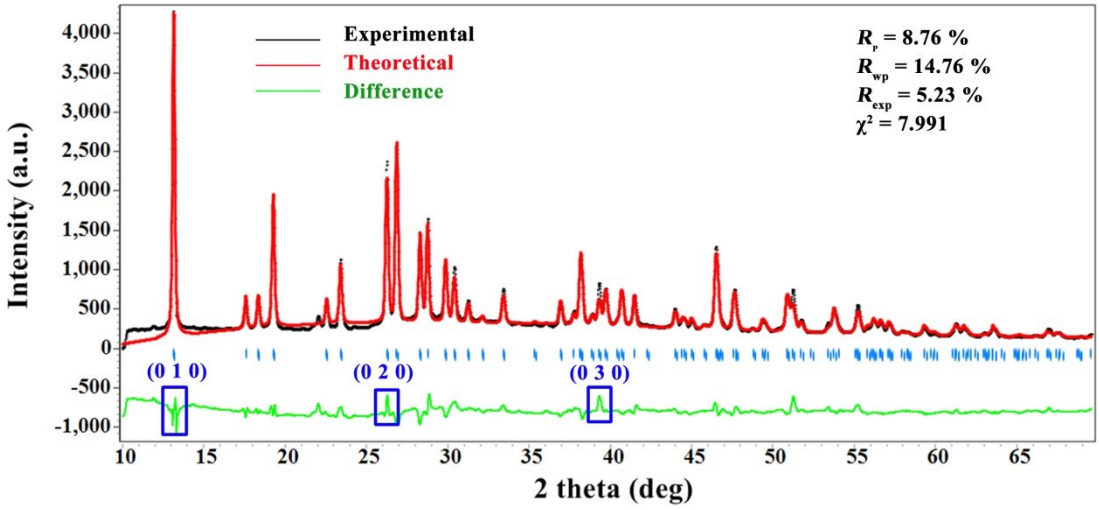

Fig. S3. The energy dispersive X-ray spectroscopy of Li_2CdSiS_4.