Supporting Information

$LiSr_3Be_3B_3O_9F_4$: A New Ultraviolet Nonlinear Optical Crystal for Fourth-harmonic Generation of Nd:YAG Lasers

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Figure S1. Powder XRD patterns of $LiSr_3Be_3B_3O_9F_4$ before and after melting.

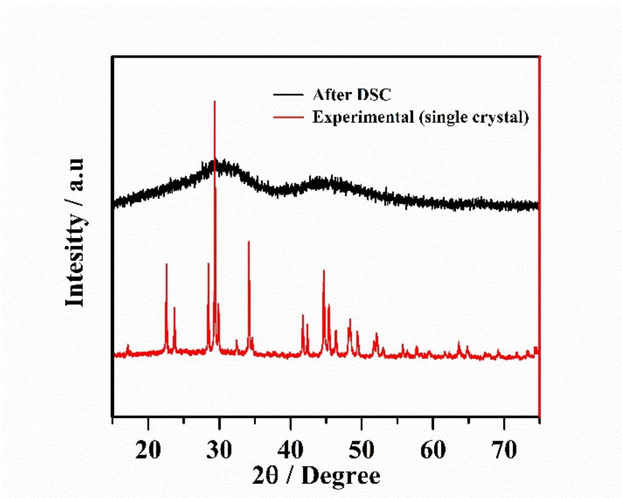

Figure S2 Calculated electronic properties in $LiSr_3Be_3B_3O_9F_4$.

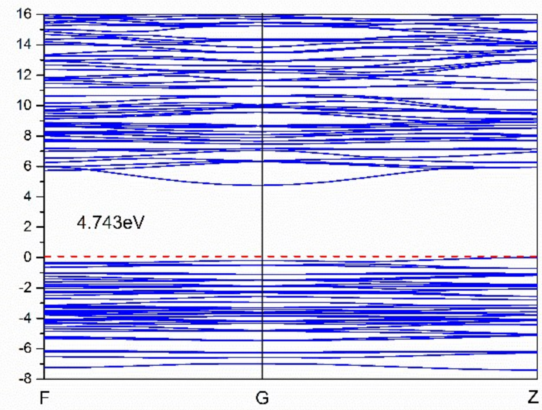

Table S1. Crystal data and structure refinement for $LiSr_3Be_3B_3O_9F_4$.

Formula	$LiSr_3Be_3B_3O_9F_4$
formula mass(amu)	549.26
crystal system	trigonal
space group	*R3m*
a(Å)	10.3062(15)
b(Å)	10.3062(15)
c(Å)	8.3458(17)
α	90
β	90
γ	120
V(Å^3)	767.7(2)
Z	3
T(K)	153.15
ρ(calcd)(g/cm^3)	3.564
λ (Å)	0.71073
F(000)	756.0
θ(deg)	3.3398-27.4855
Cryst size (mm^3)	0.26×0.24×0.24
μ(mm^{-1})	15.683
$R(F)^a$	0.0278(232)
$R_W(F_o^2)^b$	0.0651(237)

$^aR(F) = \sum \mid \mid F_o \mid - \mid F_c \mid \mid / \sum \mid F_o \mid$ for $F_o^2 > 2\sigma(F_o^2)$.

$^bR_w(F_o^2) = \{(\sum [w(F_o^2 - F_c^2)^2] / \sum wF_o^4\}^{1/2}$ for all data.

$w^{-1} = \sigma^2(F_o^2) + (zP)^2$, where $P = (_{Max}(F_o^2, 0) + 2 F_c^2)/3$.

Table S2. Selected bond lengths (Å) and bond angles for $LiSr_3Be_3B_3O_9F_4$.

Sr1–F2	2.414(7)	Be1–F1	1.546(12)
Sr1–F2	2.451(4)	O2–B1–O2	124.2(9)
Sr1–O2	2.615(4)	O2–B1–O1	117.8(4)
Sr1–O2	2.951(5)	O2–Be1–O2	108.5(8)
Sr1-O1	2.700(5)	O2–Be1–O1	110.9(6)
B1–O1	1.401(12)	O2–Be1–F1	108.7(6)
B1–O2	1.361(6)	O1–Be1–F1	108.9(9)
Be1–O1	1.533(14)	F2–Li1– F2	86.5(16)
Be1–O2	1.529(8)	F2–Li1–F1	127.7(11)
Li1–F1	2.51(5)	Be1–F1–Be1	118.9(3)
Li1–F2	2.20(3)	B1–O2–Be1	122.4(7)

Table S3. Atomic coordinates and equivalent isotropic displacement parameters for $LiSr_3Be_3B_3O_9F_4$.

Atom	Wyckoff	x/a	y/b	z/c	Ueq [Å^2]
Sr1	9b	0.06773(8)	0.53387(4)	1.0020(2)	0.0067(3)
O1	9b	0.2283(4)	0.7717(4)	0.8089(9)	0.0092(13)
O2	18c	0.2359(5)	0.9975(5)	0.8805(5)	0.0091(11)
F1	3a	1/3	2/3	0.6098(15)	0.020(2)
F2	9b	-0.1383(8)	0.4308(4)	0.8146(9)	0.0179(13)
B1	9b	0.1529(6)	0.8471(6)	0.8555(13)	0.005(2)
Be1	9b	0.2472(7)	0.7528(7)	0.6298(15)	0.003(2)
Li1	3a	-1/3	1/3	0.979(6)	0.038(10)