

Electronic Supplementary Information (ESI)

LiVTeO₅: A Mid-Infrared Nonlinear Optical Vanadium Tellurate exhibiting Enhanced Second Harmonic Generation Activities and Notable Birefringence

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Table S1. Atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for LVTO, U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor, and the bond valence sum for each atom in asymmetric unit.

Atoms	x	y	z	U_{eq}	BVS
Li(1)	9512(18)	6178(9)	-180(8)	16(2)	0.97
Te(1)	9504(1)	6883(1)	3498(1)	8(1)	3.80
V(1)	4598(1)	5222(1)	1481(1)	7(1)	5.09
O(1)	2862(6)	6727(4)	925(3)	13(1)	1.91
O(2)	3125(7)	3258(4)	824(3)	17(1)	1.92
O(3)	3643(7)	4916(4)	3112(3)	14(1)	1.69
O(4)	7832(6)	6075(4)	1868(3)	13(1)	2.17
O(5)	8427(7)	5239(4)	4663(3)	13(1)	2.46

Table S2. Selected bond lengths [\AA] and angles ($^\circ$) for LVTO.

Li(1)-O(1)#3	2.108(10)	V(1)-O(1)	1.642(3)
Li(1)-O(1)#4	2.077(8)	V(1)-O(2)	1.918(3)
Li(1)-O(3)#5	2.102(8)	V(1)-O(3)	1.650(3)
Li(1)-O(4)	2.142(8)	V(1)-O(4)	1.886(3)
Li(1)-O(5)#5	1.956(9)	V(1)-O(5)#2	2.055(3)
Te(1)-O(2)#1	1.912(3)		
Te(1)-O(4)	1.906(3)		
Te(1)-O(5)	1.852(3)		
O(5)#2-Li(1)-O(1)#6	98.6(4)	O(1)-V(1)-O(3)	104.48(17)
O(5)#2-Li(1)-O(3)#2	92.7(4)	O(1)-V(1)-O(4)	106.22(15)
O(1)#6-Li(1)-O(3)#2	107.2(3)	O(3)-V(1)-O(4)	98.71(16)
O(5)#2-Li(1)-O(1)#8	146.6(4)	O(1)-V(1)-O(2)	108.78(16)
O(1)#6-Li(1)-O(1)#8	109.8(4)	O(3)-V(1)-O(2)	92.88(14)
O(3)#2-Li(1)-O(1)#8	95.2(4)	O(4)-V(1)-O(2)	138.87(16)
O(5)#2-Li(1)-O(4)	73.6(3)	O(1)-V(1)-O(5)#2	98.94(15)
O(1)#6-Li(1)-O(4)	99.8(4)	O(3)-V(1)-O(5)#2	156.41(16)
O(3)#2-Li(1)-O(4)	151.3(4)	O(4)-V(1)-O(5)#2	77.05(13)
O(1)#8-Li(1)-O(4)	84.4(3)	O(2)-V(1)-O(5)#2	76.80(13)
O(5)-Te(1)-O(4)	94.73(14)		
O(5)-Te(1)-O(2)#1	91.13(14)		
O(4)-Te(1)-O(2)#1	98.63(14)		

Symmetry transformations used to generate equivalent atoms:

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

Table S3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for LVTO.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Li(1)	20(4)	16(3)	14(4)	2(3)	0(3)	1(4)
Te(1)	9(1)	8(1)	6(1)	0(1)	1(1)	0(1)
V(1)	7(1)	8(1)	6(1)	-1(1)	1(1)	0(1)
O(1)	9(2)	12(1)	17(2)	2(1)	1(1)	2(1)
O(2)	26(2)	14(2)	12(2)	-1(1)	5(1)	-12(2)
O(3)	19(2)	16(2)	8(2)	2(1)	-1(1)	-2(1)
O(4)	10(2)	22(2)	8(2)	-3(1)	0(1)	-2(1)
O(5)	13(2)	13(2)	13(2)	5(1)	-2(1)	-4(1)

Table S4. The magnitude (Debye) of LiO_5 , TeO_3 and VO_5 polyhedral dipole moments in LVTO.

Species	polyhedron	$X(a)$	$Y(b)$	$Z(c)$	Magnitude Debye
	LiO_5	2.2380	0.0145	-1.7990	2.8714
LVTO	TeO_3	-20.606	-7.4780	1.5948	21.9794
	VO_5	0.4360	0.6360	4.3500	4.4178

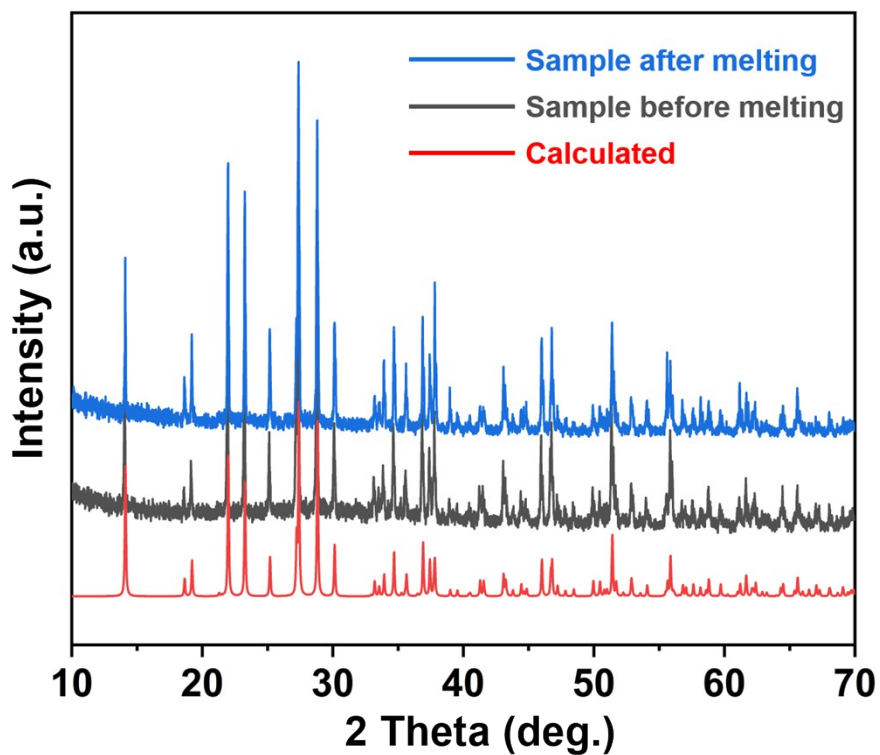


Figure S1. Powder XRD patterns of the initial and melting LVTO samples, respectively.



Figure S2. The as-grown single crystal of LVTO.

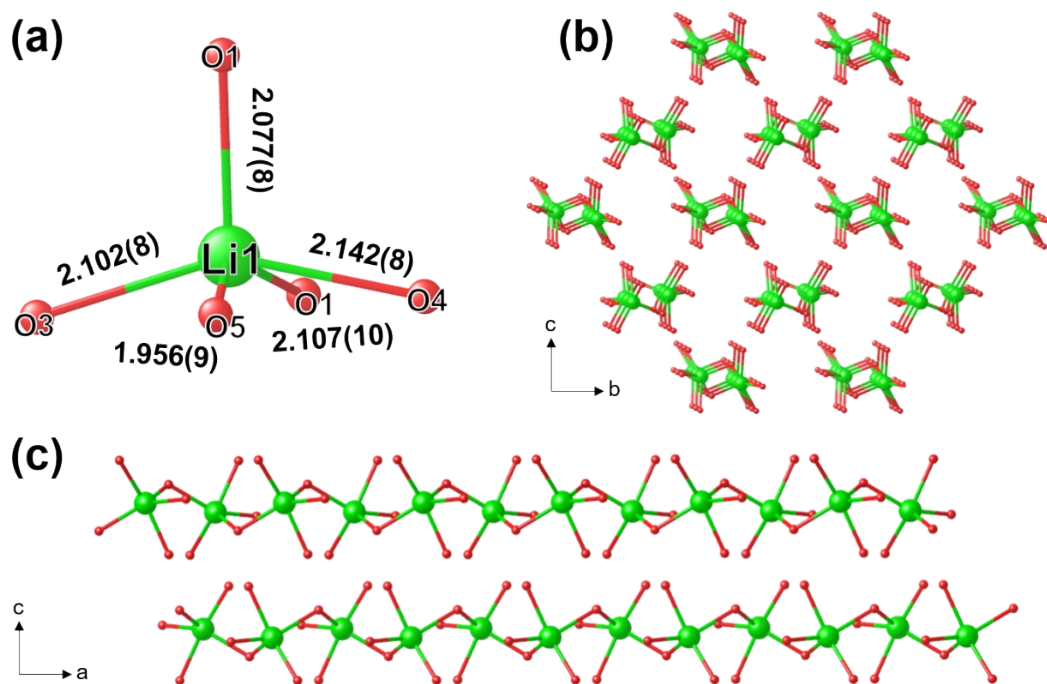


Figure S3. (a) The Li-O bond lengths [\AA] for LVTO. (b-c) The connection mode of Li atoms viewed along the bc and ac plane, respectively.

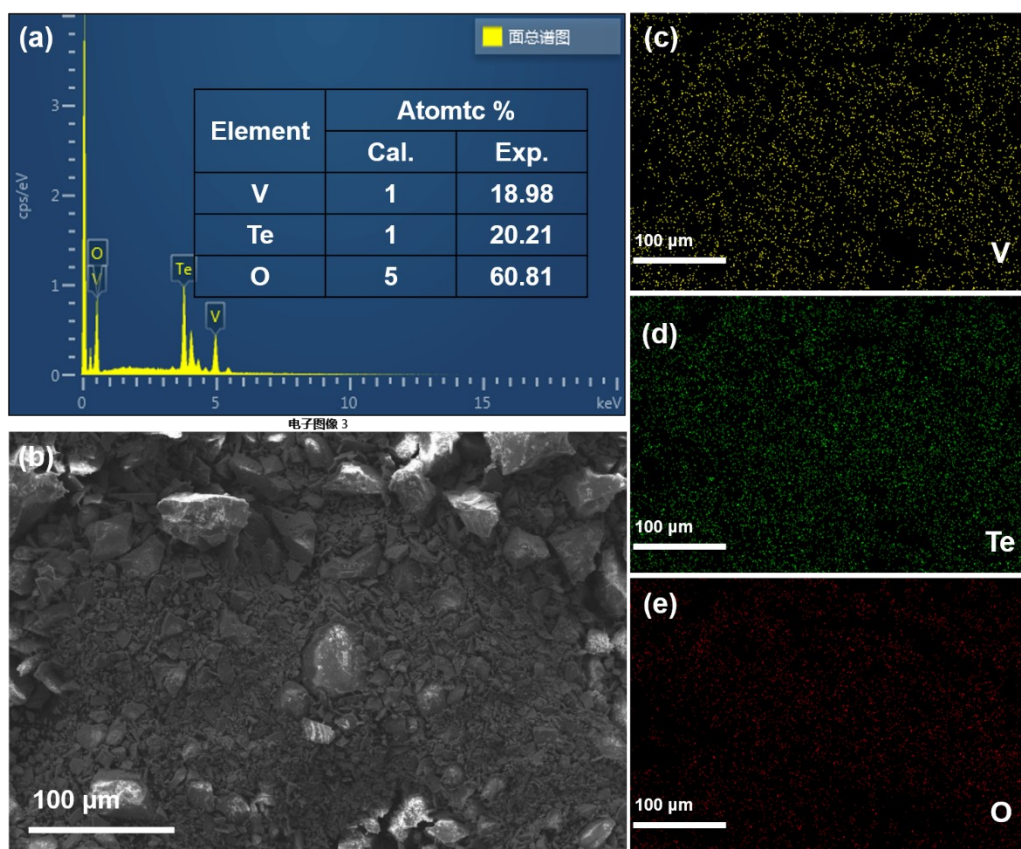


Figure S4. (a-e) Energy-dispersive spectroscopy (EDS) analysis of the LVTO crystal.

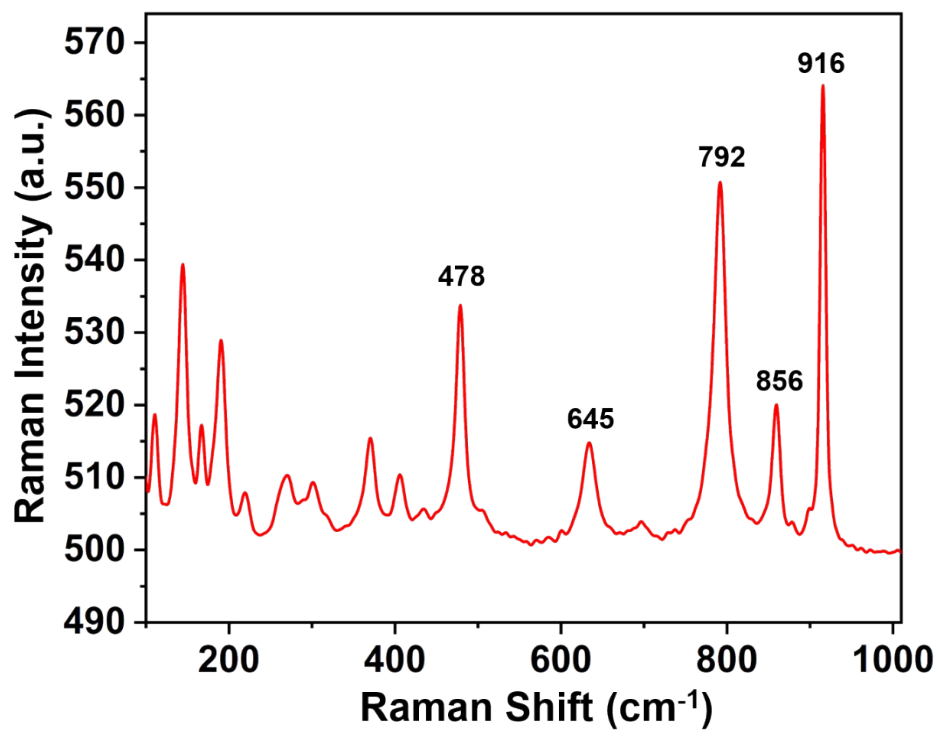


Figure S5. The Raman spectrum of the LVTO crystal.

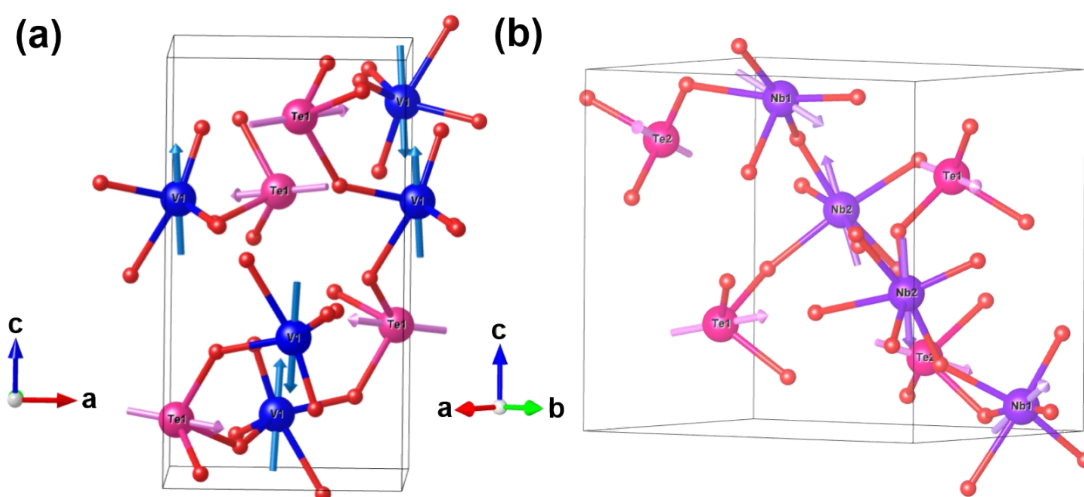


Figure S6. The orientations of the dipole moments of the anionic groups for (a) LVTO and (b) LiNbTeO_5 .