Electronic Supplementary Information (ESI)

A new stable polymorphism of $Li_2TeMo_3O_{12}$ with wide mid-infrared transparency and large Raman response

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Table S1. Atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters ($Å^2 \times 10^3$) and atomic occupancy factors for β-LTM, 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**	**OCC**
Li(1)	0	0	5000	35(9)	0.98	1
Li(2)	3350(30)	910(40)	8190(20)	32(8)	0.92	0.5
Te(1)	3333	6667	8029(1)	19(1)	3.90	1
Mo(1)	2251(1)	3136(1)	6683(1)	14(1)	6.06	1
O(1)	2583(6)	2163(7)	7486(4)	32(2)	1.96	1
O(2)	1271(6)	1888(6)	5841(4)	24(1)	2.08	1
O(3)	715(6)	3276(6)	7284(4)	16(1)	2.24	1
O(4)	3701(6)	5288(5)	7433(4)	20(1)	2.15	1

Table S2. Selected bond lengths [Å] and angles (°) for β-LTM.

Li(1)-O(2)#1	2.136(5)	Te(1)-O(4)#16	1.880(6)
Li(1)-O(2)#2	2.136(5)	Te(1)-O(4)#17	1.880(6)
Li(1)-O(2)	2.136(5)	Te(1)-O(4)	1.880(6)
Li(1)-O(2)#3	2.136(5)	Mo(1)-O(1)	1.706(6)
Li(1)-O(2)#4	2.136(5)	Mo(1)-O(2)	1.720(6)
Li(1)-O(2)#5	2.136(5)	Mo(1)-O(3)	1.898(5)
Li(2)-O(3)#5	1.99(3)	Mo(1)-O(3)#18	1.917(5)
Li(2)-O(1)	2.11(4)	Mo(1)-O(4)	2.268(5)
Li(2)-O(4)#12	2.13(3)	Mo(1)-O(4)#10	2.336(6)
Li(2)-O(2)#8	2.18(3)		
Li(2)-O(2)#13	2.25(3)		
Li(2)-O(1)#12	2.46(4)		
O(2)#1-Li(1)-O(2)#2	180.0(2)	O(2)#1-Li(1)-O(2)#4	89.4(2)
O(2)#1-Li(1)-O(2)	90.6(2)	O(2)#2-Li(1)-O(2)#4	90.6(2)
O(2)#2-Li(1)-O(2)	89.4(2)	O(2)-Li(1)-O(2)#4	90.6(2)
O(2)#1-Li(1)-O(2)#3	89.4(2)	O(2)#3-Li(1)-O(2)#4	89.4(2)
O(2)#2-Li(1)-O(2)#3	90.6(2)	O(2)#1-Li(1)-O(2)#5	90.6(2)
O(2)-Li(1)-O(2)#3	180	O(2)#2-Li(1)-O(2)#5	89.4(2)
O(2)-Li(1)-O(2)#5	89.4(2)	O(3)#5-Li(2)-O(1)	94.0(13)
O(2)#3-Li(1)-O(2)#5	90.6(2)	O(3)#5-Li(2)-O(4)#12	109.2(14)
O(2)#4-Li(1)-O(2)#5	180.0(3)	O(1)-Li(2)-O(4)#12	92.2(12)
O(4)#16-Te(1)-O(4)#17	99.7(2)	O(3)#5-Li(2)-O(2)#8	80.1(11)
O(4)#16-Te(1)-O(4)	99.7(2)	O(1)-Li(2)-O(2)#8	103.4(15)
O(4)#17-Te(1)-O(4)	99.7(2)	O(4)#12-Li(2)-O(2)#8	161.4(17)

O(1)-Mo(1)-O(2)	106.1(3)	O(3)#5-Li(2)-O(2)#13	164.9(16)
O(1)-Mo(1)-O(3)	98.4(3)	O(1)-Li(2)-O(2)#13	96.0(13)
O(2)-Mo(1)-O(3)	101.2(2)	O(4)#12-Li(2)-O(2)#13	81.7(11)
O(1)-Mo(1)-O(3)#18	100.6(3)	O(2)#8-Li(2)-O(2)#13	86.6(10)
O(2)-Mo(1)-O(3)#18	95.1(2)	O(3)#5-Li(2)-O(1)#12	86.8(13)
O(3)-Mo(1)-O(3)#18	150.4(3)	O(1)-Li(2)-O(1)#12	168.2(16)
O(1)-Mo(1)-O(4)	90.7(3)	O(4)#12-Li(2)-O(1)#12	76.5(11)
O(2)-Mo(1)-O(4)	162.0(3)	O(2)#8-Li(2)-O(1)#12	88.3(11)
O(3)-Mo(1)-O(4)	82.2(2)	O(2)#13-Li(2)-O(1)#12	85.7(11)
O(3)#18-Mo(1)-O(4)	75.1(2)		
O(1)-Mo(1)-O(4)#10	164.6(3)		
O(2)-Mo(1)-O(4)#10	88.6(2)		
O(3)-Mo(1)-O(4)#10	73.8(2)		
O(3)#18-Mo(1)-O(4)#10	82.2(2)		
O(4)-Mo(1)-O(4)#10	75.2(3)		

Symmetry transformations used to generate equivalent atoms:

#1 y,-x+y,-z+1	#2 -y,x-y,z	#3 -x,-y,-z+1
#4 x-y,x,-z+1	#5 -x+y,-x,z	#6 -x+y+1/3,-x+2/3,z-1/3
#7 x-y-1/3,x-2/3,-z+4/3	#8 -x+2/3,-y+1/3,-z+4/3	#9 x-2/3,y-1/3,z-1/3
#10 y-1/3,-x+y+1/3,-z+4/3	#11 -y+1/3,x-y-1/3,z-1/3	#12 x-y+1/3,x-1/3,-z+5/3
#13 -y+2/3,x-y+1/3,z+1/3	#14 y+1/3,-x+y+2/3,-z+5/3	#15 -x+1/3,-y+2/3,-z+5/3
#16 -x+y,-x+1,z	#17 -y+1,x-y+1,z	#18 x-y+2/3,x+1/3,-z+4/3
#19 x+2/3,y+1/3,z+1/3	#20 x-y+1/3,x+2/3,-z+5/3	

Table S3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for β-LTM.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Li(1)	35(13)	35(13)	30(20)	0	0	17(7)
Li(2)	15(14)	40(18)	34(17)	-23(14)	-9(12)	8(13)
Te(1)	23(1)	23(1)	11(1)	0	0	12(1)
Mo(1)	14(1)	10(1)	19(1)	-1(1)	-3(1)	6(1)
O(1)	28(3)	37(4)	39(4)	22(3)	12(3)	22(3)
O(2)	19(3)	16(3)	31(3)	-9(2)	3(2)	5(2)
O(3)	13(2)	15(3)	21(3)	5(2)	4(2)	7(2)
O(4)	15(3)	10(3)	36(3)	4(2)	-3(2)	6(2)

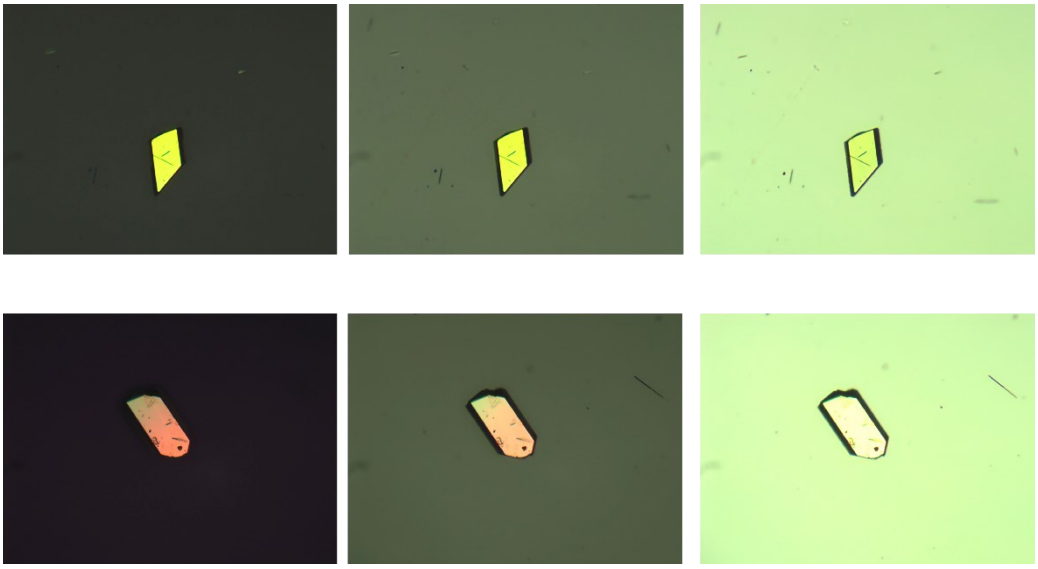

Figure S1. Single crystal pictures of α-LTM in polarizing microscope.

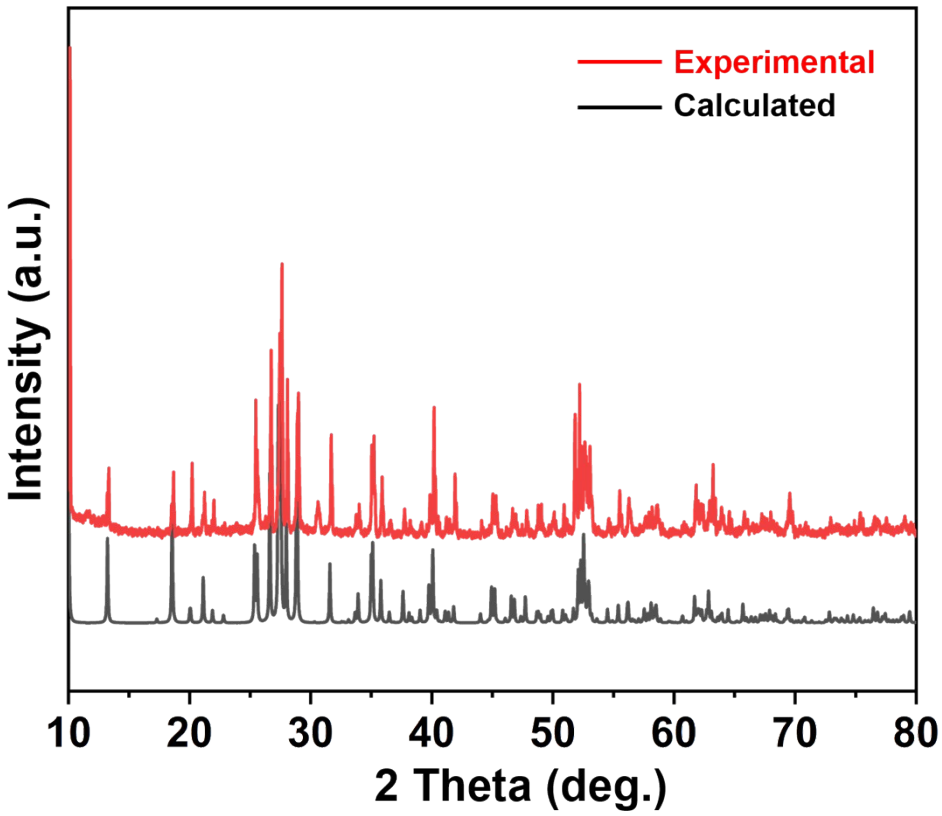

Figure S2. Calculated and experimental PXRD patterns for polycrystalline α-LTM.

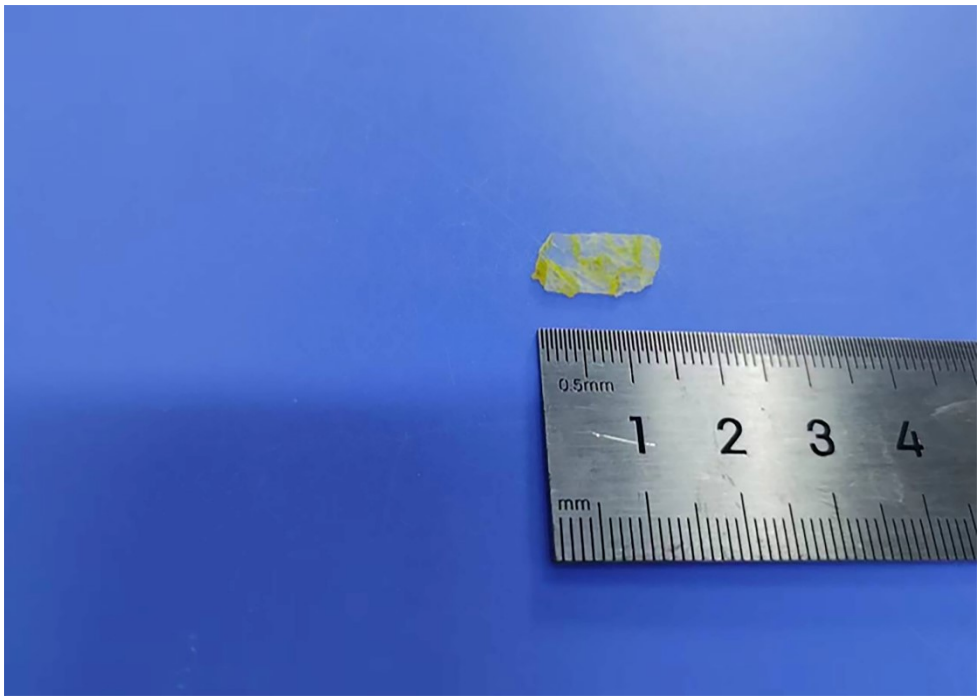

Figure S3. large-sized β-LTM crystal cultivated by the top-seeded solution growth method.

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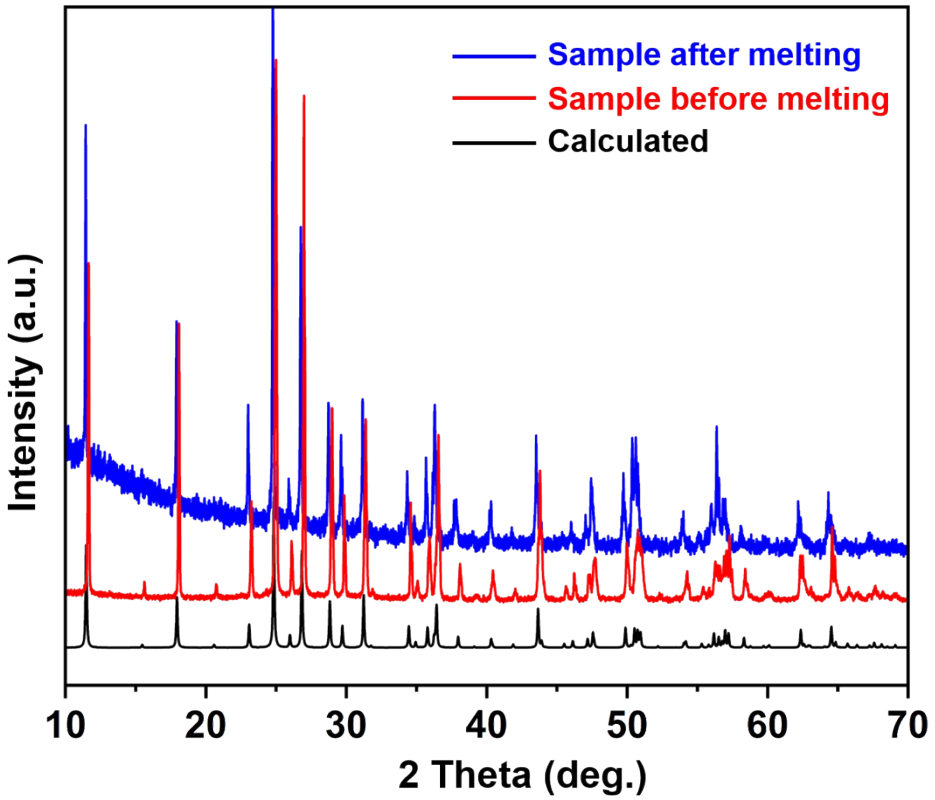

Figure S4. Powder XRD patterns of the initial and melting β-LTM samples, respectively.

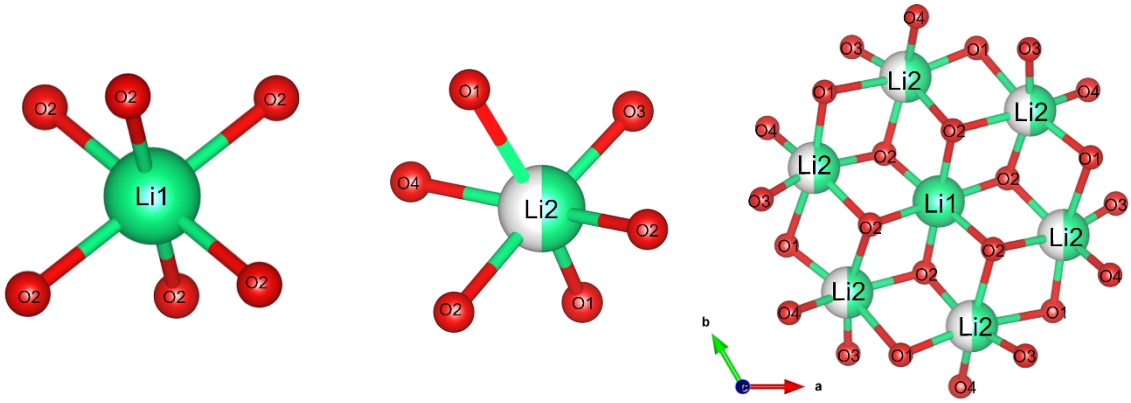

Figure S5. Coordination environment and connection mode of Li1 and Li2 atoms in β-LTM.

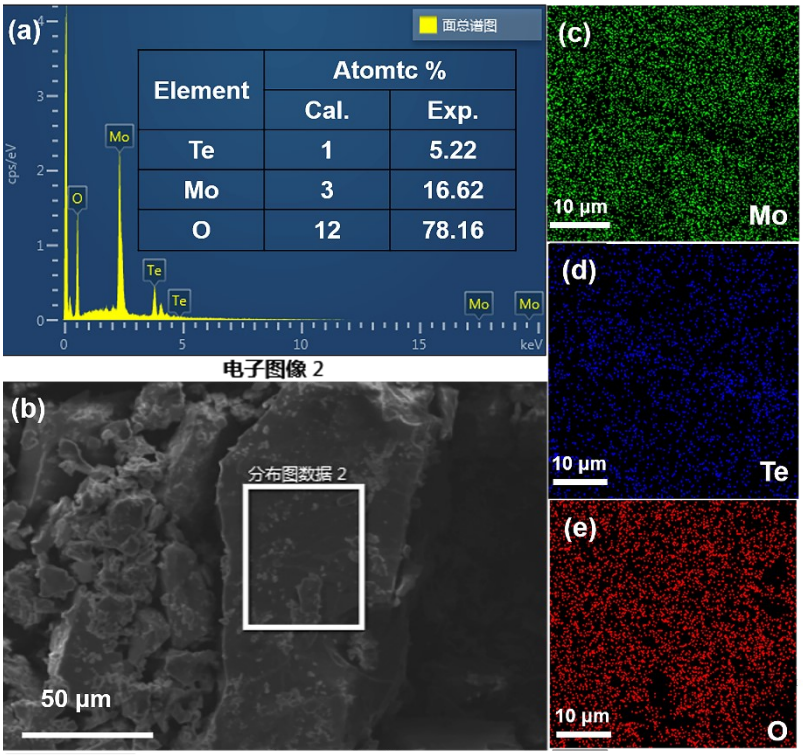

Figure S6. (a-e) Energy-dispersive spectroscopy (EDS) analysis of the β-LTM crystal.

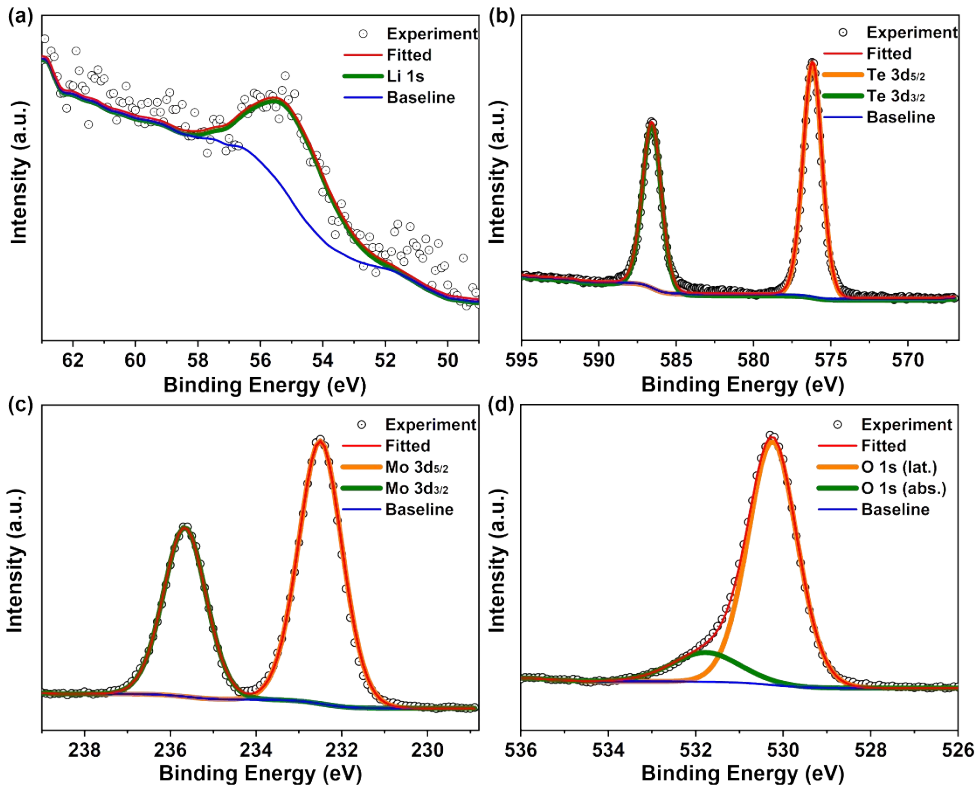

Figure S7. (a-d) X-ray photoelectron spectrum (XPS) for *β*-LTM crystal.