The study of electrochemical Li-ion (de)insertion in the lithium tantalum phosphate bronze $LiTa_2PO_8$ structure

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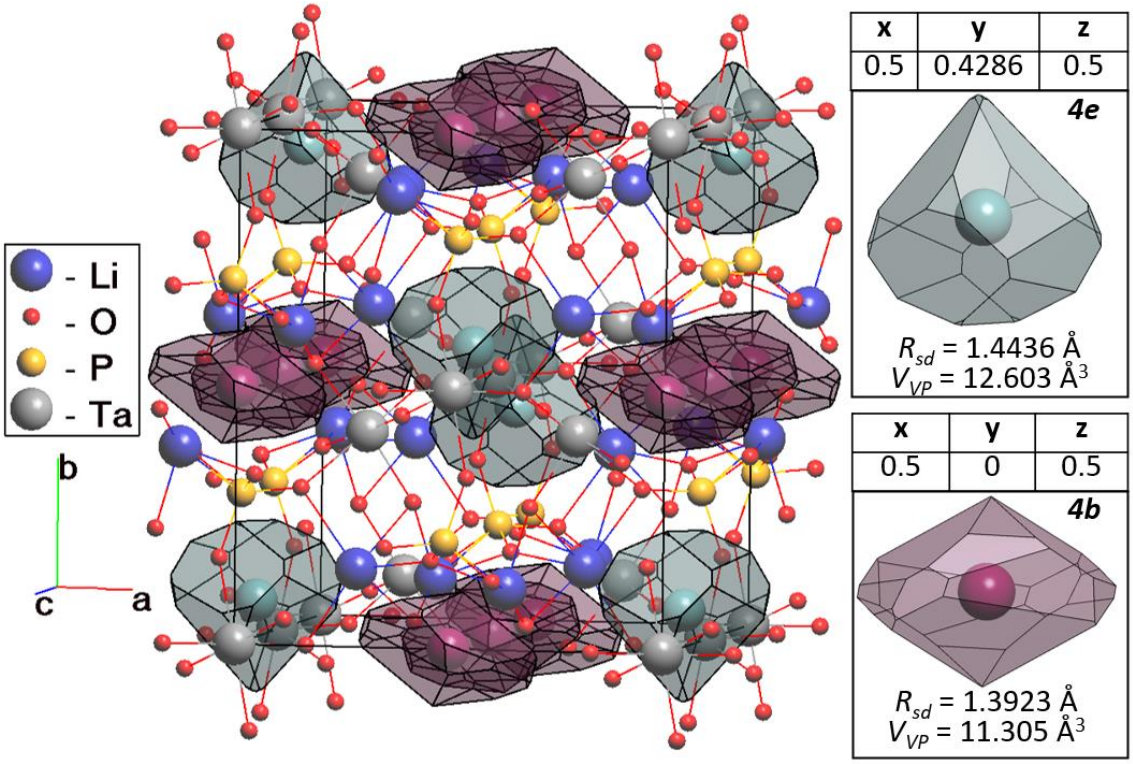

Fig. S1. Possible voids for Li placement in $LiTa_2PO_8$ with the indicated Wyckoff position, the volume of the Voronoi polyhedron volume (V_{VP}) and the radius of the spherical domain (R_{sd}).

Table S1. The occupancies of Li atom positions in the 13 $Li_{1+x}Ta_2PO_8$ structures with the given number of generated 1×1×1 configurations using the Supercell program for quantum-chemical modeling.

$Li_{1+x}Ta_2PO_8$	Variant	Position	Occupancy	Number of configurations	Composition
x = 0	1	*8f*	0.625	784	$Li_8Ta_{16}P_8O_{64}$
		8f	0.25		
		4b	0.25		
x = 0.5	1	*8f*	1.00	28	$Li_{12}Ta_{16}P_8O_{64}$
		8f	0.375		
		4b	0.25		
	2	*8f*	0.375	1	
		8f	1.00		
		4b	0.25		
	3	*8f*	0.625	784	
		8f	0.25		
		4b	0.25		
		4e	1.00		
	4	*8f*	0.625	392	
		8f	0.25		
		4b	0.25		
		4b	1.00		
x = 1	1	*8f*	1.00	4	$Li_{16}Ta_{16}P_8O_{64}$
		8f	0.875		
		4b	0.25		
	2	*8f*	0.875	4	
		8f	1.00		
		4b	0.25		
	3	*8f*	1.00	28	
		8f	0.375		
		4b	0.25		
		4e	1.00		
	4	*8f*	0.375	28	
		8f	1.00		
		4b	0.25		
		4e	1.00		
	5	*8f*	1.00	14	
		8f	0.375		
		4b	0.25		
		4b	1.00		
	6	*8f*	0.375	14	
		8f	1.00		
		4b	0.25		
		4b	1.00		
	7	*8f*	0.625	392	
		8f	0.25		
		4b	0.25		
		4e	1.00		
		4b	1.00		
x = 1.5	1	*8f*	1.00	1	$Li_{20}Ta_{16}P_8O_{64}$
		8f	1.00		
		4b	1.00		

Table S2. DFT-derived energies of simple atoms included in $Li_{1+x}Ta_2PO_8$.

Element	Li	Ta	P	O
E_{iso}, eV/f.u.	-1.9077	-11.8513	-5.4057	-4.9524

Table S3. Total energy of the cell and with the number of formula units, cohesive energy and lithium vacancy formation energy from the DFT data in $Li_{1+x}Ta_2PO_8$.

Composition	E_{total}, eV	E_{total}, eV/f.u.	E_{coh}, eV/f.u.	E_v, eV
$Li_8Ta_{16}P_8O_{64}$	-819.3197	-102.4150	**-31.7798***	1.83
$Li_{12}Ta_{16}P_8O_{64}$ (#1)	-830.8381	-103.8548	-32.2658	0.39
$Li_{12}Ta_{16}P_8O_{64}$ (#2)	-831.0498	-103.8812	-32.2922	0.37
$Li_{12}Ta_{16}P_8O_{64}$ (#3)	-829.5573	-103.6947	-32.1057	0.55
$Li_{12}Ta_{16}P_8O_{64}$ (#4)	-831.5097	-103.9387	**-32.3497**	0.31
$Li_{16}Ta_{16}P_8O_{64}$ (#1)	-841.5107	-105.1888	-32.6459	0.94
$Li_{16}Ta_{16}P_8O_{64}$ (#2)	-842.0507	-105.2563	**-32.7134**	1.01
$Li_{16}Ta_{16}P_8O_{64}$ (#3)	-839.9775	-104.9972	-32.4543	0.75
$Li_{16}Ta_{16}P_8O_{64}$ (#4)	-840.3912	-105.0489	-32.5060	0.80
$Li_{16}Ta_{16}P_8O_{64}$ (#5)	-841.8915	-105.2364	-32.6935	0.99
$Li_{16}Ta_{16}P_8O_{64}$ (#6)	-840.7371	-105.0921	-32.5492	0.84
$Li_{16}Ta_{16}P_8O_{64}$ (#7)	-840.4979	-105.0622	-32.5193	0.81
$Li_{20}Ta_{16}P_8O_{64}$	-849.2527	-106.1566	**-32.6599**	-

* - the cohesive energies for the most stable configurations are highlighted in bold

Table S4 Rietveld refined lattice parameters of the $LiTa_2PO_8$

Space Group	*C2/c*
a, Å	9.7195(2)
b, Å	11.5397(5)
c, Å	10.7020(1)
β, ^{o}	89.990(3)
V, Å^3	1200.338(2)
GOF	2.7
R_p, %	4.8
R_{wp}, %	6.7
Wt%	95.8

Table S5 Atomic coordinates for $LiTa_2PO_8$

Atom	Wyckoff	*x/a*	*y/b*	*z/c*	Occupancy	B_{iso}
Ta1	8f	0.2459(3)	0.0965(2)	0.2620(4)	1	0.3395
Ta2	4a	0.0	0.3470(3)	0.25	1	0.3079
Ta3	4e	0.0	0.0	0.0	1	0.2921
P1	8f	0.4843(29)	0.1998(13)	0.0502(12)	1	0.5606
O1	8f	0.0336(40)	0.3354(31)	0.0863(28)	1	1.224
O2	8f	0.3500(35)	0.1329(33)	0.4272(34)	1	1.042
O3	8f	0.4323(38)	0.4923(33)	0.1093(31)	1	1.271
O4	8f	0.0391(41)	0.1936(29)	0.5604(27)	1	1.05
O5	8f	0.1648(28)	0.2195(25)	0.2807(41)	1	0.8133
O6	8f	0.1445(48)	0.0371(38)	0.1256(34)	1	1.469
O7	8f	0.3951(41)	0.1917(33)	0.1465(27)	1	1.319
O8	8f	0.1608(31)	0.4909(28)	0.2951(32)	1	1.358
Li1	8f	0.2450	0.3570	0.1400	0.72	1.658
Li2	8f	0.1120	0.3870	0.4000	0.21	1.658
Li3	4b	0.5	0.0	0.0	0.14	1.658

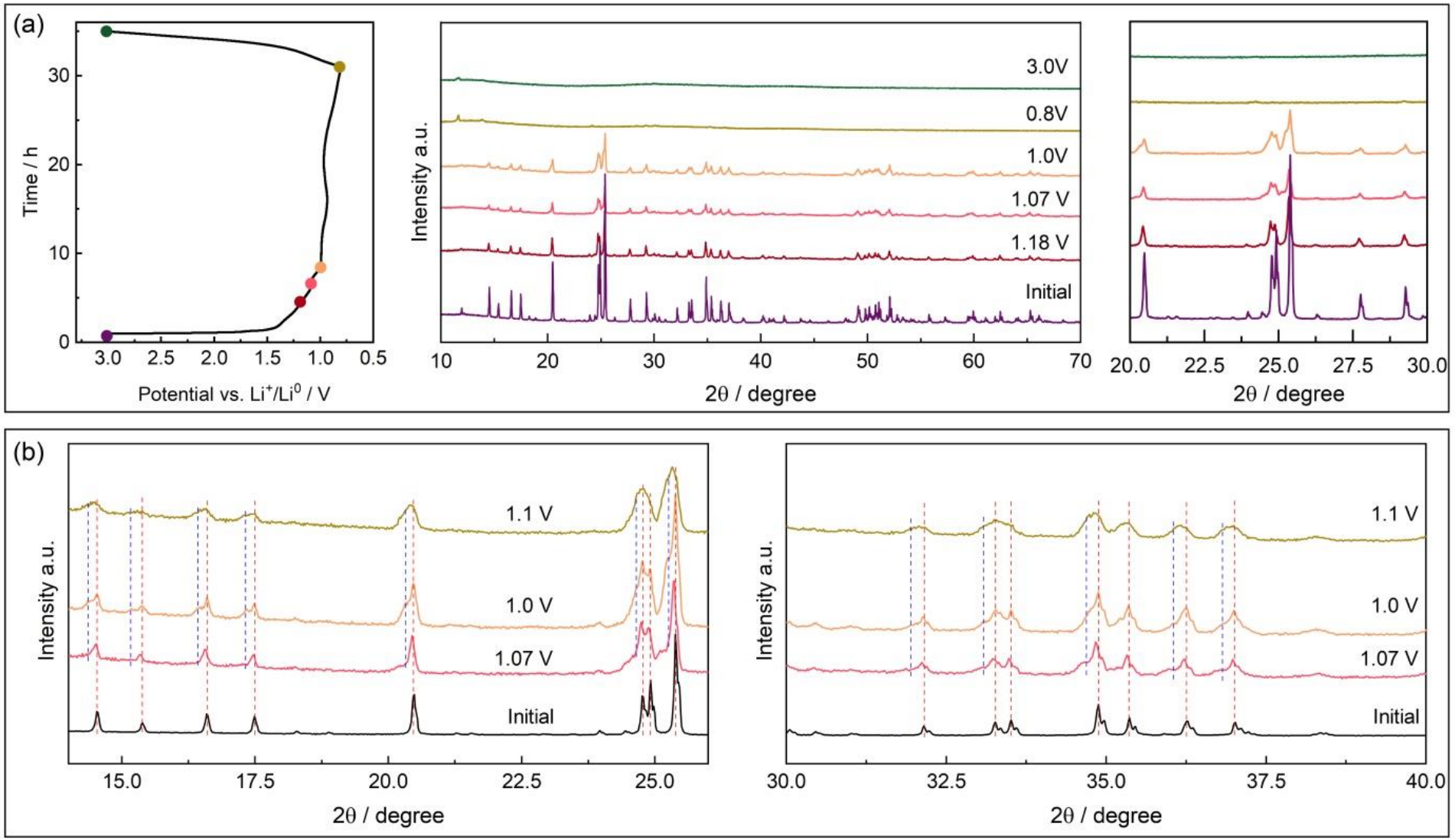

Fig. S2. *Ex situ* XRD data for $LiTa_2PO_8$ cycled in 0.8-3.0 V (a) and 1.0-3.0 V potential ranges (b)