

Supporting information.

Unusual Mn coordination and redox chemistry in the high capacity borate cathode $\text{Li}_7\text{Mn}(\text{BO}_3)_3$

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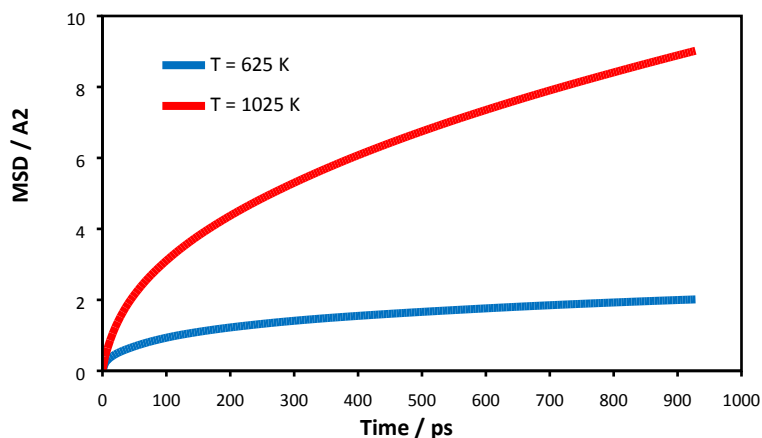


Figure S1 Mean squared displacement (MSD) of lithium ions for $\text{Li}_{6.3}\text{Mn}(\text{BO}_3)_3$ over ≈ 0.9 ns at 625 K (blue) and 1025 K (red).

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cif-File of lithiated DFT optimised structure $\text{Li}_7\text{Mn}(\text{BO}_3)_3$

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CRYSTAL DATA

20 data_VESTA_phase_1

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_pd_phase_name      'B3 Li7 Mn1 O9'
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25 _cell_length_b    9.19348
   _cell_length_c    11.21641
   _cell_angle_alpha 71.63880
   _cell_angle_beta  79.68598
   _cell_angle_gamma 71.39971
30 _symmetry_space_group_name_H-M 'P 1'
   _symmetry_Int_Tables_number     1

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loop_
_symmetry_equiv_pos_as_xyz
35 'x, y, z'

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loop_						
_atom_site_label						
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_atom_site_fract_z						
_atom_site_adp_type						
_atom_site_B_iso_or_equiv						
10	_atom_site_type_symbol					
	Mn1	1.0	0.296071	0.474158	0.579512	Biso 1.000000 Mn
	Mn2	1.0	0.703332	0.525754	0.420126	Biso 1.000000 Mn
	Mn3	1.0	0.458820	0.393623	0.157279	Biso 1.000000 Mn
	Mn4	1.0	0.539119	0.606237	0.841340	Biso 1.000000 Mn
15	O1	1.0	0.149539	0.363099	0.723857	Biso 1.000000 O
	O2	1.0	0.849862	0.636614	0.275808	Biso 1.000000 O
	O3	1.0	0.016597	0.682103	0.079998	Biso 1.000000 O
	O4	1.0	0.984367	0.317071	0.920509	Biso 1.000000 O
	O5	1.0	0.045407	0.572789	0.829769	Biso 1.000000 O
20	O6	1.0	0.953065	0.427317	0.169382	Biso 1.000000 O
	O7	1.0	0.099626	0.825241	0.258219	Biso 1.000000 O
	O8	1.0	0.899892	0.174891	0.740956	Biso 1.000000 O
	O9	1.0	0.005329	0.033156	0.363921	Biso 1.000000 O
	O10	1.0	0.993829	0.967394	0.634736	Biso 1.000000 O
25	O11	1.0	0.173579	0.075147	0.168586	Biso 1.000000 O
	O12	1.0	0.825817	0.924978	0.830142	Biso 1.000000 O
	O13	1.0	0.114581	0.253339	0.478672	Biso 1.000000 O
	O14	1.0	0.884655	0.747061	0.520484	Biso 1.000000 O
	O15	1.0	0.220068	0.486243	0.409729	Biso 1.000000 O
30	O16	1.0	0.779003	0.514175	0.590097	Biso 1.000000 O
	O17	1.0	0.331429	0.271715	0.309837	Biso 1.000000 O
	O18	1.0	0.669502	0.728451	0.690519	Biso 1.000000 O
	O19	1.0	0.341329	0.380405	0.014101	Biso 1.000000 O
	O20	1.0	0.656914	0.619985	0.984083	Biso 1.000000 O
35	O21	1.0	0.424605	0.625884	0.146014	Biso 1.000000 O
	O22	1.0	0.574842	0.373687	0.853148	Biso 1.000000 O
	O23	1.0	0.555886	0.838398	0.079642	Biso 1.000000 O
	O24	1.0	0.443876	0.160967	0.919668	Biso 1.000000 O
	O25	1.0	0.520533	0.290738	0.609934	Biso 1.000000 O
40	O26	1.0	0.478924	0.709044	0.389262	Biso 1.000000 O
	O27	1.0	0.630230	0.062481	0.524632	Biso 1.000000 O
	O28	1.0	0.369286	0.937646	0.474048	Biso 1.000000 O
	O29	1.0	0.725663	0.295594	0.430327	Biso 1.000000 O
	O30	1.0	0.273657	0.704570	0.568814	Biso 1.000000 O
45	O31	1.0	0.315038	0.005408	0.740116	Biso 1.000000 O
	O32	1.0	0.684625	0.994385	0.258779	Biso 1.000000 O
	O33	1.0	0.711292	0.259398	0.148337	Biso 1.000000 O
	O34	1.0	0.287114	0.740733	0.850114	Biso 1.000000 O
	O35	1.0	0.821327	0.046857	0.049450	Biso 1.000000 O
50	O36	1.0	0.178427	0.952658	0.949545	Biso 1.000000 O
	B1	1.0	0.059119	0.422267	0.825670	Biso 1.000000 B
	B2	1.0	0.940528	0.577376	0.174001	Biso 1.000000 B
	B3	1.0	0.093768	0.975551	0.262109	Biso 1.000000 B
	B4	1.0	0.905577	0.024711	0.736779	Biso 1.000000 B
55	B5	1.0	0.220319	0.339453	0.399467	Biso 1.000000 B
	B6	1.0	0.779473	0.660744	0.600266	Biso 1.000000 B
	B7	1.0	0.548095	0.696654	0.070187	Biso 1.000000 B
	B8	1.0	0.451090	0.303075	0.928729	Biso 1.000000 B

	B9	1.0	0.621094	0.216172	0.520738	Biso	1.000000	B	
	B10	1.0	0.378249	0.783932	0.478238	Biso	1.000000	B	
	B11	1.0	0.733889	0.101808	0.152354	Biso	1.000000	B	
	B12	1.0	0.265397	0.898071	0.846393	Biso	1.000000	B	
5	Li1	1.0	0.007243	0.654288	0.384059	Biso	1.000000	Li	
	Li2	1.0	0.992155	0.345809	0.615016	Biso	1.000000	Li	
	Li3	1.0	0.036112	0.108266	0.034110	Biso	1.000000	Li	
	Li4	1.0	0.963700	0.890126	0.965147	Biso	1.000000	Li	
	Li5	1.0	0.056954	0.845608	0.512964	Biso	1.000000	Li	
10	Li6	1.0	0.942801	0.154259	0.485854	Biso	1.000000	Li	
	Li7	1.0	0.107420	0.161799	0.809789	Biso	1.000000	Li	
	Li8	1.0	0.892237	0.837872	0.189640	Biso	1.000000	Li	
	Li9	1.0	0.159733	0.296506	0.110190	Biso	1.000000	Li	
	Li10	1.0	0.834974	0.705045	0.882698	Biso	1.000000	Li	
15	Li11	1.0	0.200311	0.759819	0.100999	Biso	1.000000	Li	
	Li12	1.0	0.799256	0.240135	0.898529	Biso	1.000000	Li	
	Li13	1.0	0.200052	0.044099	0.592071	Biso	1.000000	Li	
	Li14	1.0	0.799806	0.956221	0.406249	Biso	1.000000	Li	
	Li15	1.0	0.213271	0.110251	0.348269	Biso	1.000000	Li	
20	Li16	1.0	0.786303	0.891563	0.648345	Biso	1.000000	Li	
	Li17	1.0	0.324334	0.656202	0.305961	Biso	1.000000	Li	
	Li18	1.0	0.675390	0.343356	0.693451	Biso	1.000000	Li	
	Li19	1.0	0.348410	0.007413	0.040834	Biso	1.000000	Li	
	Li20	1.0	0.651731	0.991809	0.958391	Biso	1.000000	Li	
25	Li21	1.0	0.405771	0.169733	0.755076	Biso	1.000000	Li	
	Li22	1.0	0.594283	0.829592	0.244261	Biso	1.000000	Li	
	Li23	1.0	0.506647	0.078229	0.379934	Biso	1.000000	Li	
	Li24	1.0	0.493142	0.921752	0.618677	Biso	1.000000	Li	
	Li25	1.0	0.827999	0.419808	0.042434	Biso	1.000000	Li	
30	Li26	1.0	0.170202	0.581250	0.956627	Biso	1.000000	Li	
	Li27	1.0	0.845274	0.266841	0.272608	Biso	1.000000	Li	
	Li28		1.0	0.152838	0.733141	0.726393	Biso	1.000000	Li

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cif-File of delithiated DFT optimised structure $\text{Li}_4\text{Mn}(\text{BO}_3)_3$

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CRYSTAL DATA

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50 data_VESTA_phase_1

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	_cell_length_c	11.86226
	_cell_angle_alpha	71.48025
	_cell_angle_beta	77.90579

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_cell_angle_gamma          75.10814
_symmetry_space_group_name_H-M    'P 1'
_symmetry_Int_Tables_number      1

5 loop_
_symmetry_equiv_pos_as_xyz
  'x, y, z'

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    _atom_site_occupancy
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
15  _atom_site_adp_type
    _atom_site_B_iso_or_equiv
    _atom_site_type_symbol
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Mn2  1.0  0.644506  0.513844  0.432553  Biso 1.000000 Mn
20  Mn3  1.0  0.412515  0.391769  0.143628  Biso 1.000000 Mn
Mn4  1.0  0.541553  0.645885  0.836072  Biso 1.000000 Mn
O1   1.0  0.215840  0.280748  0.753685  Biso 1.000000 S
O2   1.0  0.802971  0.624242  0.304456  Biso 1.000000 S
O3   1.0  -0.037942  0.706270  0.112443  Biso 1.000000 O
25  O4   1.0  0.961706  0.284194  0.921385  Biso 1.000000 O
O5   1.0  0.025180  0.517143  0.765725  Biso 1.000000 O
O6   1.0  0.865831  0.461765  0.161436  Biso 1.000000 O
O7   1.0  0.099935  0.830042  0.271684  Biso 1.000000 O
O8   1.0  0.849320  0.193552  0.698366  Biso 1.000000 O
30  O9   1.0  0.011054  0.065479  0.345433  Biso 1.000000 O
O10  1.0  -0.005145  0.956139  0.638691  Biso 1.000000 O
O11  1.0  0.200283  0.067713  0.163491  Biso 1.000000 O
O12  1.0  0.894692  0.958271  0.846319  Biso 1.000000 O
O13  1.0  0.221028  0.232899  0.512859  Biso 1.000000 S
35  O14  1.0  0.873004  0.751694  0.507499  Biso 1.000000 O
O15  1.0  0.208698  0.496933  0.404196  Biso 1.000000 S
O16  1.0  0.684101  0.559964  0.571495  Biso 1.000000 S
O17  1.0  0.312294  0.290251  0.297458  Biso 1.000000 S
O18  1.0  0.697704  0.715715  0.695279  Biso 1.000000 S
40  O19  1.0  0.388051  0.460131  -0.020949  Biso 1.000000 S
O20  1.0  0.627480  0.642066  0.982286  Biso 1.000000 S
O21  1.0  0.386300  0.612621  0.146405  Biso 1.000000 S
O22  1.0  0.610991  0.428242  0.825095  Biso 1.000000 S
O23  1.0  0.562674  0.804682  0.118191  Biso 1.000000 O
45  O24  1.0  0.515377  0.190124  0.950274  Biso 1.000000 O
O25  1.0  0.511528  0.355860  0.551524  Biso 1.000000 S
O26  1.0  0.445908  0.701915  0.406317  Biso 1.000000 S
O27  1.0  0.603068  0.081387  0.525444  Biso 1.000000 O
O28  1.0  0.303959  0.879842  0.526037  Biso 1.000000 O
50  O29  1.0  0.736079  0.309130  0.407052  Biso 1.000000 S
O30  1.0  0.239889  0.619047  0.584364  Biso 1.000000 S
O31  1.0  0.251798  0.108922  0.751338  Biso 1.000000 O
O32  1.0  0.690644  0.992225  0.273620  Biso 1.000000 O
O33  1.0  0.653628  0.263753  0.137382  Biso 1.000000 S
55  O34  1.0  0.383575  0.849142  0.797826  Biso 1.000000 S
O35  1.0  0.834657  0.035686  0.076810  Biso 1.000000 O
O36  1.0  0.256775  0.954330  0.968890  Biso 1.000000 O
B1   1.0  0.053807  0.358943  0.820913  Biso 1.000000 B

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	B4	1.0	0.920359	0.031346	0.726963	Biso	1.000000	B
	B5	1.0	0.247649	0.335799	0.398310	Biso	1.000000	B
5	B6	1.0	0.752406	0.678378	0.587659	Biso	1.000000	B
	B7	1.0	0.527264	0.688744	0.080813	Biso	1.000000	B
	B8	1.0	0.501240	0.348886	0.919957	Biso	1.000000	B
	B9	1.0	0.615552	0.232007	0.499116	Biso	1.000000	B
	B10	1.0	0.331068	0.730700	0.508081	Biso	1.000000	B
10	B11	1.0	0.719385	0.098615	0.163167	Biso	1.000000	B
	B12	1.0	0.298627	0.968021	0.851683	Biso	1.000000	B
	Li1	1.0	-0.007494	0.655113	0.389995	Biso	1.000000	Li
	Li2	1.0	0.066682	0.094361	0.028976	Biso	1.000000	Li
	Li3	1.0	0.105230	0.059502	0.484901	Biso	1.000000	Li
15	Li4	1.0	0.889152	0.844832	0.215218	Biso	1.000000	Li
	Li5	1.0	0.182089	0.754670	0.066201	Biso	1.000000	Li
	Li6	1.0	0.790402	0.164464	0.908654	Biso	1.000000	Li
	Li7	1.0	0.389664	0.010488	0.604392	Biso	1.000000	Li
	Li8	1.0	0.783655	0.970241	0.428304	Biso	1.000000	Li
20	Li9	1.0	0.308225	0.670277	0.294994	Biso	1.000000	Li
	Li10	1.0	0.650947	0.359153	0.684280	Biso	1.000000	Li
	Li11	1.0	0.412916	0.015202	0.043816	Biso	1.000000	Li
	Li12	1.0	0.807045	0.850652	0.002980	Biso	1.000000	Li
	Li13	1.0	0.565322	0.838658	0.272531	Biso	1.000000	Li
25	Li14	1.0	0.810553	0.426669	0.024857	Biso	1.000000	Li
	Li15	1.0	0.857416	0.262754	0.268441	Biso	1.000000	Li
	Li16	1.0	0.005332	0.730526	0.657742	Biso	1.000000	Li