**Supporting information**

Cathode properties, average and electronic structures of αLi2MnO3–

(1−*α*)Li(Mn10/24Ni7/24Co7/24)O2 in Li-ion batteries with TiNb2O7 anode.

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グラフ

自動的に生成された説明

Fig. S1 Crystal structure model (space group: *C*2/*m*)

Li3

Li2

Li1

カラフルな凧を飛ばしている人のイラスト

低い精度で自動的に生成された説明

Li4

図形

自動的に生成された説明

Li 1~4

Fig. S2 Crystal structure model (space group: *C*2/*m*)



Fig. S3 Rietveld refinement of the synchrotron X-ray diffraction pattern for 05LMNC//TNO after the 5th discharge (TNO) (space group *C*2/*m*).

Table S1 Final results of Rietveld refinements for 05LMNC//TNO after the 5th discharge (TNO).

*R*-factor: *R*wp = 10.9%, *R*p = 8.66*%*, *R*e = 2.17*%*

*a* = 2.03821(7) nm, *b* = 0.380269(9) nm, *c* = 1.190170(4) nm, *β =* 120.213(9) deg.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Atoms | Site | *x* | *y* | *z* | 102×*B* (nm2) | Site Occupancy |
| Ti1 | *2a* | 0 | 0 | 0 | 1.70413 | 0.1717 |
| Nb1 | *2a* | =Ti1(*x*) | =Ti1(*y*) | =Ti1(*z*) | =Ti1(β) | 0.8282 |
| Ti2 | *4i* | 0.1854 | 0 | 0.005084 | 0.6958 | 0.1636 |
| Nb2 | *4i* | =Ti2(*x*) | =Ti2(*y*) | =Ti2(*z*) | =Ti2(β) | 0.8363 |
| Ti3 | *4i* | 0.07759 | 0 | 0.6361 | 0.6151 | 0.3271 |
| Nb3 | *4i* | =Ti3(*x*) | =Ti3(*y*) | =Ti3(*z*) | =Ti3(β) | 0.6728 |
| Ti4 | *4i* | 0.8910 | 0 | 0.6325 | 0.1788 | 0.2996 |
| Nb4 | *4i* | =Ti4(*x*) | =Ti4(*y*) | =Ti4(*z*) | =Ti4(β) | 0.7003 |
| Ti5 | *4i* | 0.2933 | 0 | 0.3671 | 0.7257 | 0.6237 |
| Nb5 | *4i* | =Ti5(*x*) | =Ti5(*y*) | =Ti5(*z*) | =Ti5(β) | 0.3762 |
| O1 | *2b* | 0.1709 | 0 | 0.5928 | 0.144798 | 1 |
| O2 | *4i* | 0.3726 | 0 | 0.5852 | 0.144798 | 1 |
| O3 | *4i* | 0.6012 | 0 | 0.6223 | 0.144798 | 1 |
| O4 | *4i* | 0.7901 | 0 | 0.6132 | 0.144798 | 1 |
| O5 | *4i* | 0.2420 | 0 | 0.1837 | 0.144798 | 1 |
| O6 | *4i* | 0.7077 | 0 | 0.8862 | 0.144798 | 1 |
| O7 | *4i* | 0.9064 | 0 | 0.9897 | 0.144798 | 1 |
| O8 | *4i* | 0.0226 | 0 | 0.4092 | 0.144798 | 1 |
| O9 | *4i* | 0.8722 | 0 | 0.1813 | 0.144798 | 1 |
| O10 | *4i* | 0 | 0.5 | 0 | 0.144798 | 1 |
| O11 | *4i* | 0.05411 | 0 | 0.2027 | 0.144798 | 1 |
| Li1 | *4i* | 0.2566 | 0 | 0.7971 | 0.01721 | 0.2835 |
| Li2 | *4i* | 0.1598 | 0 | 0.1841 | 0.01100 | 0.2835 |
| Li3 | *4i* | 0.04454 | 0 | 0.8244 | 0.01122 | 0.2835 |
| Li4 | *4i* | 0.2926 | 0 | 0.6088 | 0.01100 | 0.2835 |

Table S2 Bond lengths for *M*O6 octahedra in the transition-metal layer, as obtained by Rietveld analysis.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Sample | | Pristine(05LMNC) | 05LMNC//Li | | 05LMNC//TNO | |
|  | site |  | 5th charge | 5th discharge | 5th charge | 5th discharge |
| *d*(nm) | *4g-4i* | 0.19980(5) | 0.19834(8) | 0.19458(9) | 0.19750(3) | 0.19809(9) |
| *4g-8j* | 0.19959(5) | 0.19059(7) | 0.20303(7) | 0.20712(2) | 0.19455(4) |
| *2b-4i* | 0.18979(9) | 0.18435(8) | 0.20925(4) | 0.19428(6) | 0.19701(6) |
| *2b-8j* | 0.18667(2) | 0.18462(4) | 0.18853(4) | 0.18098(3) | 0.18209(5) |
| Sample | | Pristine(04LMNC) | 04LMNC//Li | | 04LMNC//TNO | |
|  | site |  | 5th charge | 5th discharge | 5th charge | 5th discharge |
| *d*(nm) | *4g-4i* | 0.20089(6) | 0.20209(1) | 0.19693(1) | 0.19739(8) | 0.20032(5) |
| *4g-8j* | 0.20158(2) | 0.20267(4) | 0.20246(2) | 0.20203(6) | 0.20162(3) |
| *2b-4i* | 0.19089(9) | 0.18613(3) | 0.18692(5) | 0.21333(7) | 0.19578(7) |
| *2b-8j* | 0.18801(7) | 0.18234(7) | 0.19703(6) | 0.17525(6) | 0.19849(5) |

Table S3 BVS parameters in the transition-metal layer and Li layer, as obtained by Rietveld analysis for each sample.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Sample | | Pristine | 05LMNC//Li | | 05LMNC//TNO | |
|  | site |  | 5th charge | 5th discharge | 5th charge | 5th discharge |
| BVS | *4g* | 3.279 | 3.282 | 3.114 | 3.266 | 3.252 |
| *2b* | 2.153 | 4.112 | 2.692 | 3.802 | 2.532 |
| *2c* | 1.081 | 1.577 | 1.032 | 1.492 | 1.104 |
| *4h* | 1.099 | 1.170 | 1.112 | 1.082 | 1.065 |
| Sample | | Pristine | 04LMNC//Li | | 04LMNC//TNO | |
|  | site |  | 5th charge | 5th discharge | 5th charge | 5th discharge |
| BVS | *4g* | 3.143 | 3.188 | 3.095 | 3.215 | 3.145 |
| *2b* | 2.477 | 3.814 | 2.877 | 3.244 | 2.641 |
| *2c* | 0.904 | 1.421 | 1.001 | 1.297 | 0.943 |
| *4h* | 0.956 | 1.023 | 0.972 | 1.005 | 1.012 |