**Supplementary Information for "$LiMg_{0.1}Co_{0.9}BO_3$ as a Positive Electrode Material for Li-ion Batteries"**

The Rietveld refinement has been performed with GSAS-II[1] based on the structure reported by Piffard *et al.*[2] The occupancy for Mg is set to 0.1 and estimated to take only Co1 positions. The atomic coordinates are also left according to the crystal structure reported by Piffard *et al.*[2] and no attempts to refine specific atomic positions are taken here. The results are given below:

## Refinement output

**Crystal data**

| | |
|---|---|
| Formula sum | B $Co_{0.9}$ Li $Mg_{0.1}$ $O_3$ |
| Formula weight | 121.22 |
| Crystal system | monoclinic |
| Space group | *C* 1 2/c 1 (no. 15) |
| Unit cell dimensions | *a* = 5.1101(6) Å |
| | *b* = 8.7962(8) Å |
| | *c* = 10.0351(9) Å |
| | β = 91.44(1) ° |
| Cell volume | 450.93(6) $Å^3$ |
| Z | 8 |
| Density, calculated | 3.571 $g/cm^3$ |
| Pearson code | mC64 |
| Formula type | NOPQ3 |
| Wyckoff sequence | $f^8$ |

**Atomic coordinates**

| Atom | Wyck. | Occ. | x | y | z |
|---|---|---|---|---|---|
| Co1 | 8*f* | 0.46 | 0.16570 | 0.16730 | 0.13250 |
| Co2 | 8*f* | 0.44 | 0.15470 | 0.16450 | 0.11360 |
| Li1 | 8*f* | 0.48 | 0.66100 | 0.00300 | 0.08800 |
| Li2 | 8*f* | 0.52 | 0.66300 | -0.00500 | 0.15700 |
| B1 | 8*f* | | 0.16420 | -0.16840 | 0.12580 |
| O1 | 8*f* | | 0.40260 | 0.33560 | 0.09130 |
| O2 | 8*f* | | -0.21670 | 0.19440 | 0.15870 |
| O3 | 8*f* | | 0.30880 | -0.03890 | 0.12660 |
| Mg9 | 8*f* | 0.1 | 0.16570 | 0.16730 | 0.13250 |

**Anisotropic displacement parameters (in $Å^2$)**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.00760 | 0.01020 | 0.00820 | 0.00010 | -0.00090 | 0.00090 |
| O2 | 0.00650 | 0.00600 | 0.01000 | 0.00020 | -0.00190 | 0.00040 |
| O3 | 0.00590 | 0.00600 | 0.04000 | 0.00010 | -0.00310 | 0.00000 |

**Selected geometric parameters (Å, °)**

| | | | |
|---|---|---|---|
| Co1—$Li2^{i}$ | 8.709(13) | Li2—$Mg9^{iv}$ | 10.622(1) |
| Co1—O1 | 1.963(3) | B1—O3 | 1.358(0) |
| Co1—O2 | 1.993(3) | O1—Co1 | 1.963(3) |
| Co1—$O2^{ii}$ | 2.118(3) | O1—Co2 | 1.983(2) |
| Co1—O3 | 1.957(0) | O2—Co1 | 1.993(3) |
| Co2—$Li1^{iii}$ | 8.641(13) | O2—$Co1^{ii}$ | 2.118(3) |
| Co2—O1 | 1.983(2) | O2—Co2 | 1.980(6) |
| Co2—O2 | 1.980(6) | O2—$Li1^{v}$ | 11.428(4) |
| Co2—O3 | 1.958(1) | O2—$Li2^{v}$ | 11.468(1) |

| | | | |
|---|---|---|---|
| Li1—Co2$^{iii}$ | 8.641(13) | O3—Co1 | 1.957(0) |
| Li1—Li1$^{iii}$ | 11.163(14) | O3—Co2 | 1.958(1) |
| Li1—Li2 | 0.696(0) | O3—Li1 | 1.887(5) |
| Li1—Li2$^{iii}$ | 11.343(19) | O3—Li1$^{iii}$ | 10.568(13) |
| Li1—O2$^{iv}$ | 11.428(4) | O3—Li2 | 1.852(4) |
| Li1—O3 | 1.887(5) | O3—Li2$^{i}$ | 10.613(13) |
| Li1—O3$^{iii}$ | 10.568(13) | O3—B1 | 1.358(0) |
| Li1—Mg9 | 2.958(5) | Mg9—Li1$^{v}$ | 10.562(2) |
| Li1—Mg9$^{iv}$ | 10.562(2) | Mg9—Li1 | 2.958(5) |
| Li1—Mg9$^{iii}$ | 8.691(14) | Mg9—Li1$^{iii}$ | 8.691(14) |
| Li2—Co1$^{i}$ | 11.366(10) | Mg9—Li2$^{v}$ | 10.622(1) |
| Li2—Li1 | 0.696(0) | Mg9—Li2 | 2.964(3) |
| Li2—Li1$^{iii}$ | 11.343(19) | Mg9—Li2$^{i}$ | 8.709(13) |
| Li2—Li2$^{i}$ | 11.287(15) | Mg9—O1 | 1.963(3) |
| Li2—O2$^{iv}$ | 11.468(1) | Mg9—O2 | 1.993(3) |
| Li2—O3 | 1.852(4) | Mg9—O2$^{ii}$ | 2.118(3) |
| Li2—O3$^{i}$ | 10.106(14) | Mg9—O3 | 1.957(0) |
| Li2—Mg9 | 2.964(3) | Mg9—Mg9$^{ii}$ | 2.938(18) |

| | | | |
|---|---|---|---|
| Li1$^{iii}$—Li1—Li2 | 103.32(0) | Li2$^{i}$—Li2—O3 | 64.18(0) |
| Li1$^{iii}$—Li1—O2$^{iv}$ | 19.03(0) | O2$^{iv}$—Li2—O3 | 76.52(0) |
| Li2—Li1—O2$^{iv}$ | 91.54(0) | Li1$^{v}$—O2—Li2$^{v}$ | 3.48(0) |
| Li1$^{iii}$—Li1—O3 | 66.98(0) | Li1—O3—Li2 | 21.42(0) |
| Li2—Li1—O3 | 76.48(0) | Li1—O3—B1 | 133.19(0) |
| O2$^{iv}$—Li1—O3 | 77.79(0) | Li2—O3—B1 | 131.72(0) |
| Li1—Li2—Li2$^{i}$ | 95.27(0) | O1—Mg9—O2 | 123.34(0) |
| Li1—Li2—O2$^{iv}$ | 84.98(0) | O1—Mg9—O3 | 117.37(0) |
| Li2$^{i}$—Li2—O2$^{iv}$ | 17.42(0) | O2—Mg9—O3 | 118.9() |
| Li1—Li2—O3 | 82.1() | | |

**Symmetry codes:**
(i) -x, 1+y, 0.5-z; (ii) -x, y, 0.5-z; (iii) -x, 1-y, -z; (iv) x, 1+y, z;
(v) x, -1+y, z.

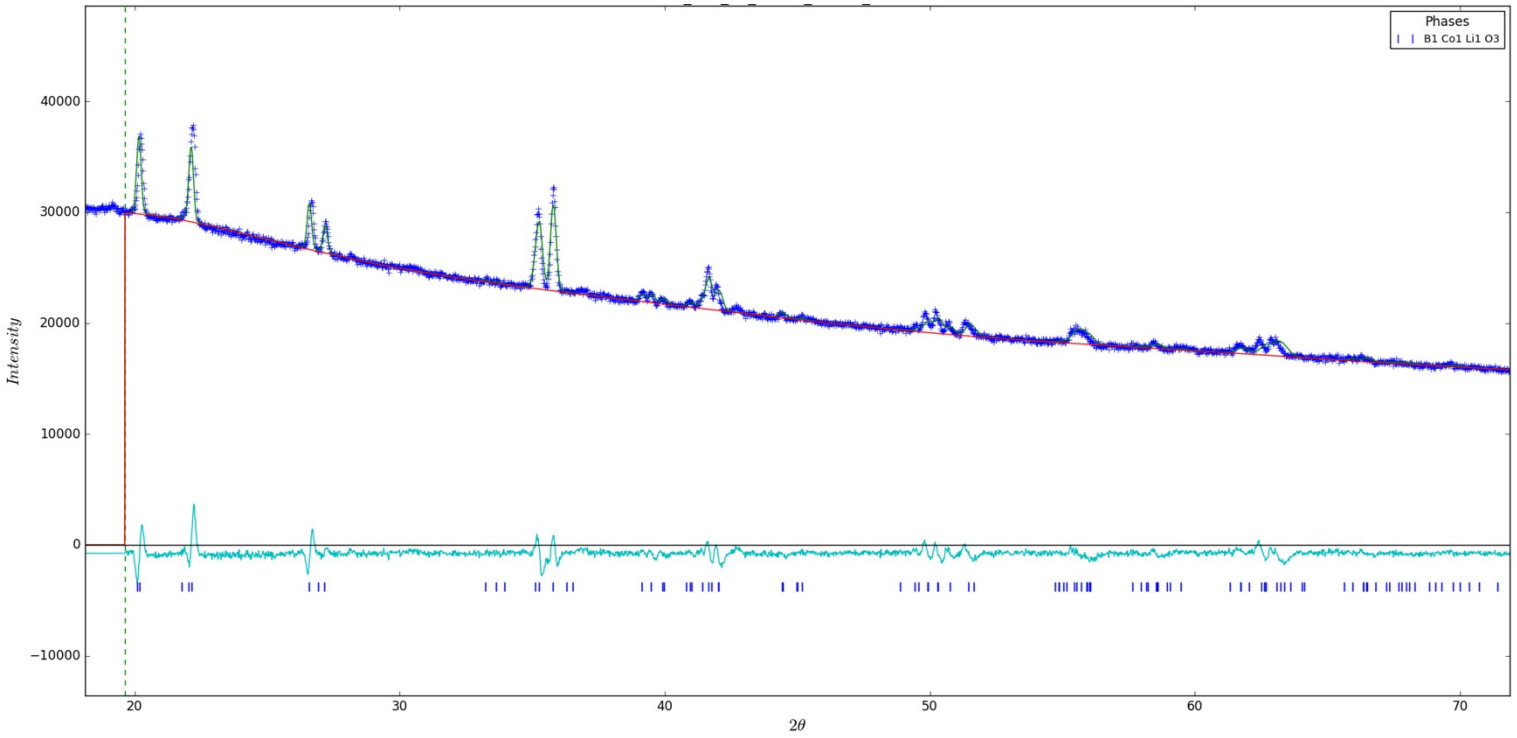


**Figure S 1** The Rietveld refinement for $LiMg_{0.1}Co_{0.9}BO_3$ (done with GSAS-II[1]) between 2 theta = 19.5 and 75 degrees, wR = 1.63 %. The blue curve corresponds to the experimental data and the green curve is the calculated fit. The bottom cyan coloured curve is the difference of the patterns, $y_{obs}$ - $y_{cal}$. The blue lines at the bottom indicate the allowed Bragg reflections.

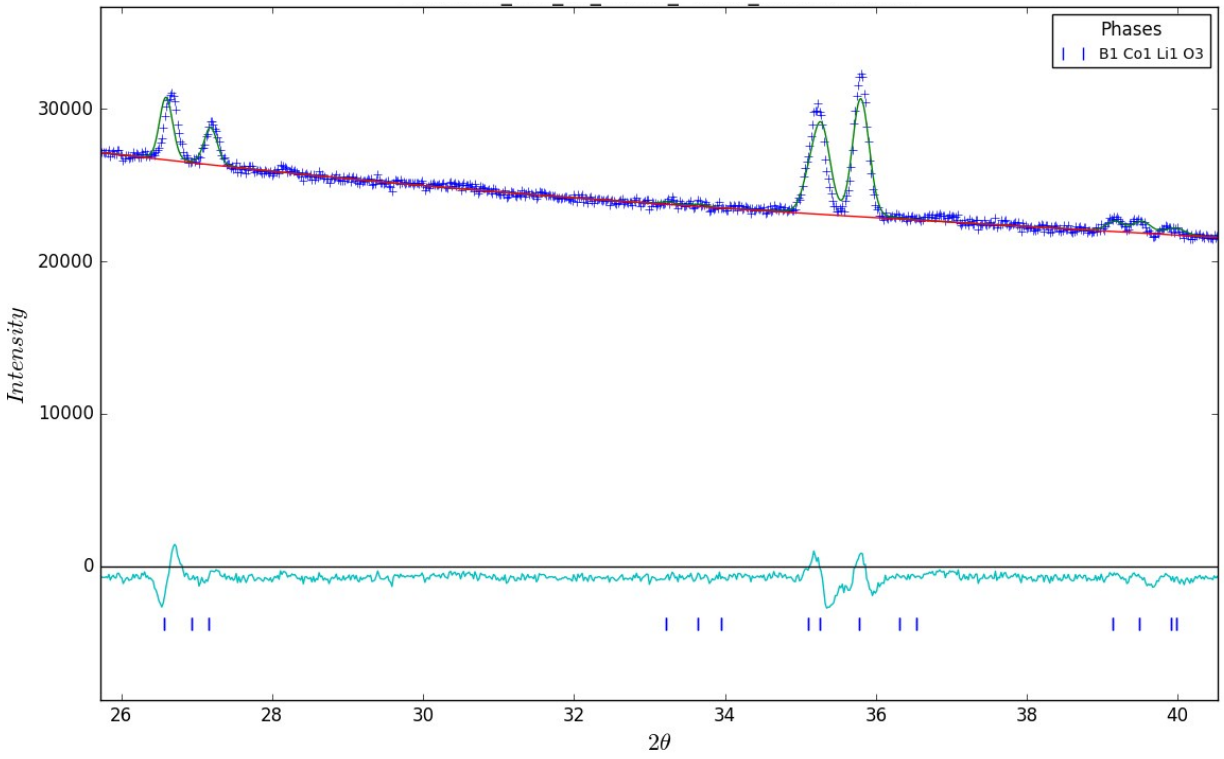


***Figure S1 Supplement*** *Zoomed in region from the refinement (Figure S1) for 2 theta = 26 and 41 degrees displaying the quality of the fit. The blue curve corresponds to the experimental data and the green curve is the calculated fit. The bottom cyan coloured curve is the difference of the patterns,* $y_{obs}$ - $y_{cal}$. *The blue lines at the bottom indicate the allowed Bragg reflections.*

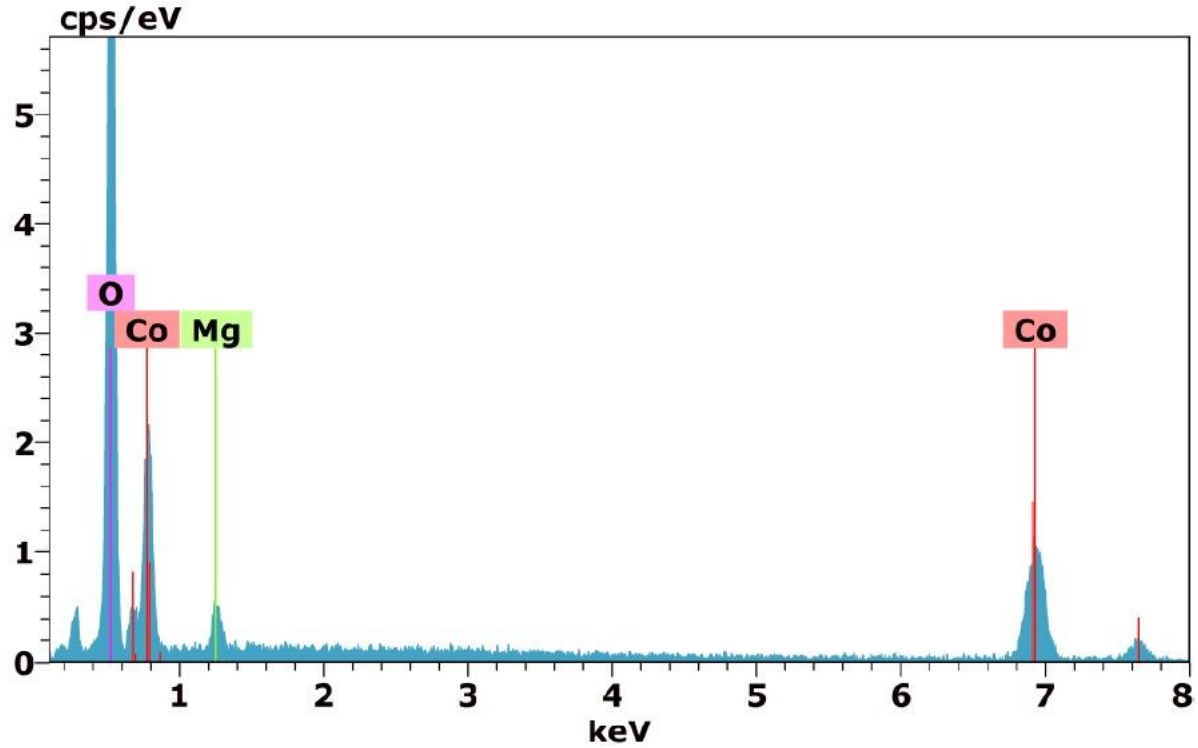


**Figure S 2** EDX analysis result showing the characteristic energies of $K_\alpha$ and $L_\alpha$ radiation of EDX detectable elements present in the active material.

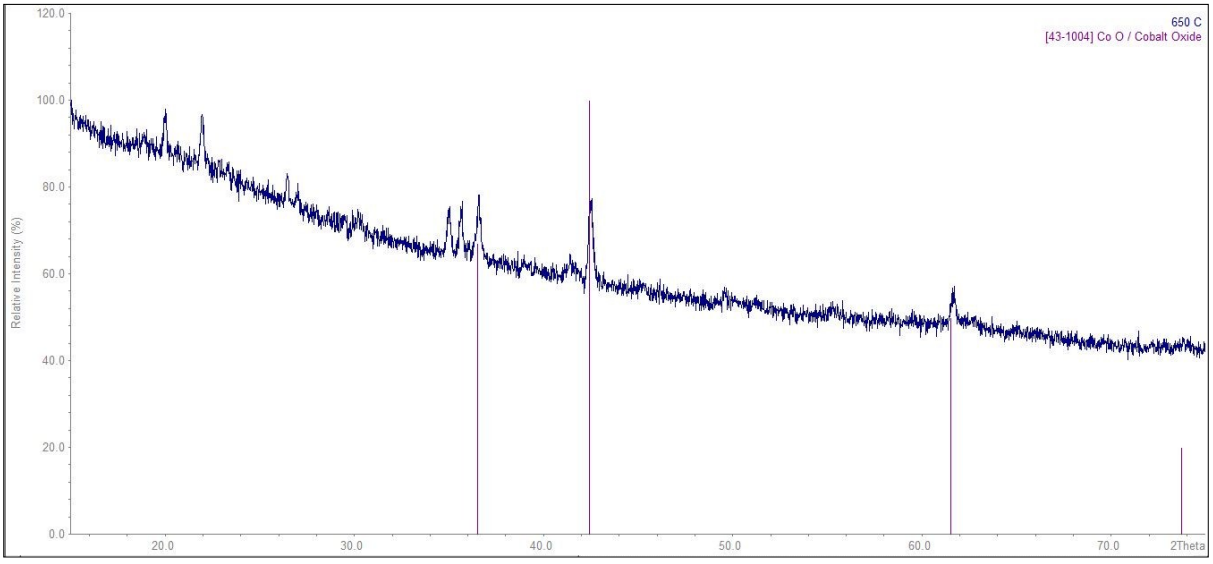


**Figure S 3** XRD powder diagram showing the presence of CoO (PDF #43-1004) impurity peaks after annealing the gel-powder at 650 °C.

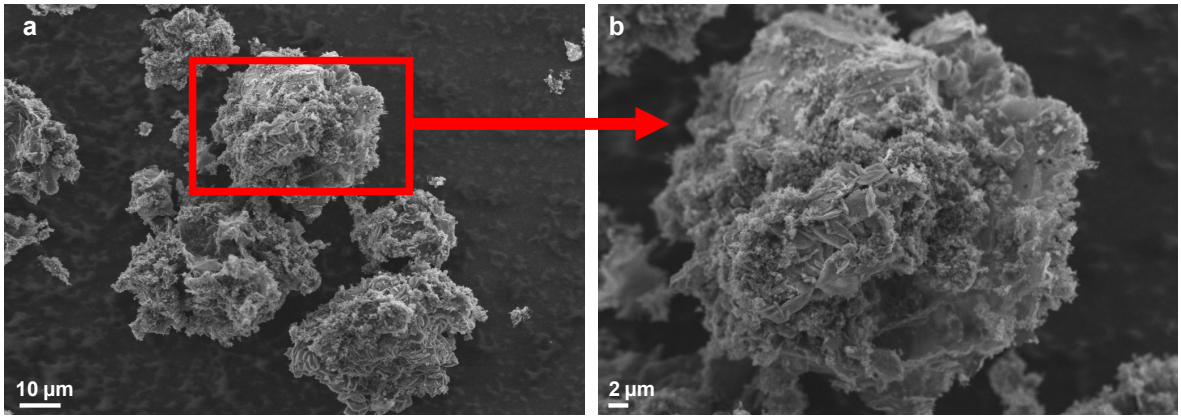


**Figure S 4** The SEM micrographs of the active material ($LiMg_{0.1}Co_{0.9}BO_3$) after mixing with conductive carbon, reduced graphite oxide, and PVDF show that the material was completely coated and had a textured surface.

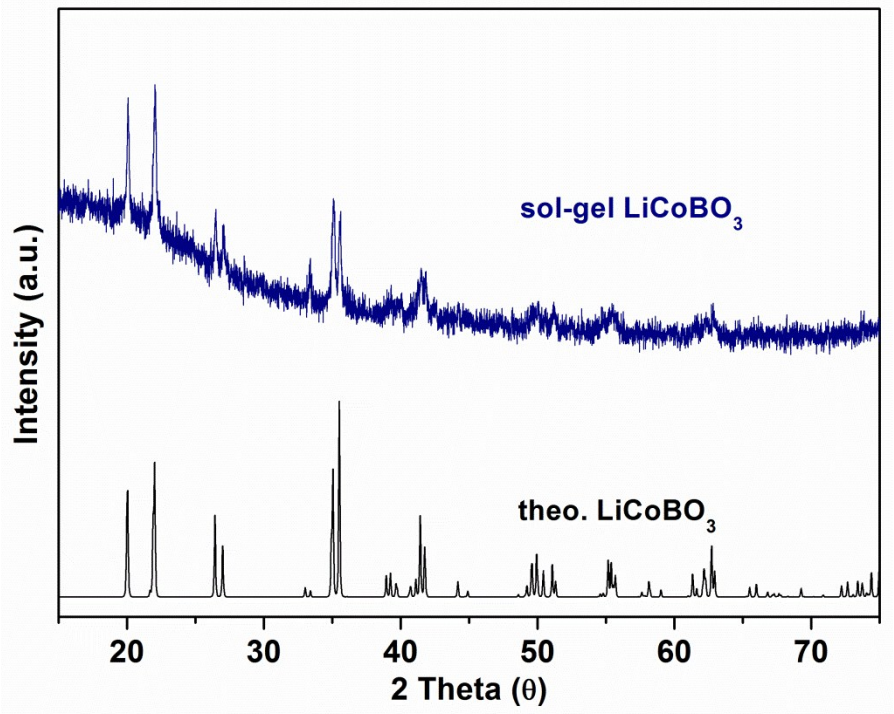


**Figure S 5** XRD powder patterns of sol-gel synthesised $LiCoBO_3$ (blue) and calculated (ICSD 59346) $LiCoBO_3$ (black).

The XRD powder pattern of the sol-gel synthesised $LiCoBO_3$ obtained in similar conditions to $LiMg_{0.1}Co_{0.9}BO_3$ (*e.g.* the gel-powder annealed above 750 °C) is shown in **Figure S5**. The experimental pattern could be directly matched to the calculated one and no obvious impurity

phases that would affect the electrochemical performance of the active material can be observed.

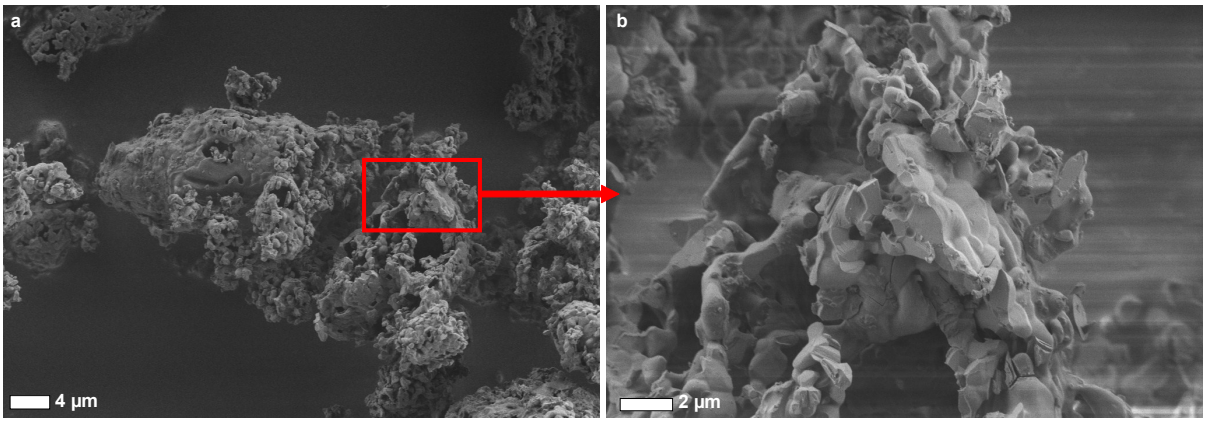


**Figure S 6** The SEM micrographs of the sol-gel synthesised $LiCoBO_3$.

The SEM micrographs of the sol-gel synthesised $LiCoBO_3$ is shown in Figure S6. The material was obtained by annealing the gel-powder at ~ 750 °C similar to the case of $LiMg_{0.1}Co_{0.9}BO_3$. The micron sized particles can be observed in the SEM images and appear form larger agglomerates.

## References

1. B. H. Toby and R. B. Von Dreele, *J Appl Crystallogr*, 2013, **46**, 544-549.
2. Y. Piffard, K. K. Rangan, Y. L. An, D. Guyomard and M. Tournoux, *Acta Crystallogr C*, 1998, **54**, 1561-1563.