Lithium storage in metal organic framework with diamondoid topology – A case study on metal formates

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Supporting Information

Gibb’s free energy calculations:

\[ \text{Zn}_3(\text{HCOO})_6 + 6 \text{Li}^+ + 6 \text{e}^- \leftrightarrow 3\text{Zn} + 6\text{HCOOLi} \text{ (reaction spontaneous)} \] \hspace{1cm} \text{equation (1)}

\[ \text{Zn(HCOO)}_2 \leftrightarrow \text{ZnO} + \text{CO} + \text{CO}_2 + \text{H}_2 \text{ (Reaction not spontaneous)} \] \hspace{1cm} \text{equation (2)}

\[ \text{Zn(HCOO)}_2 + \text{Li} \leftrightarrow \text{ZnO} + \text{Li}_2\text{O} + 2\text{CO} + \text{H}_2 \text{ (Reaction spontaneous)} \] \hspace{1cm} \text{equation (3)}

<table>
<thead>
<tr>
<th>Zinc formate (KJ/mol)</th>
<th>Lithium formate (KJ/mol)</th>
<th>$\Delta G = \Delta G_p - \Delta G_r$ (KJ/mol)</th>
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<tr>
<td>-864.8</td>
<td>-612</td>
<td>-360 KJ/mol</td>
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From this calculation it is clear that formation of lithium formate (eqn-1) is more favourable than ZnO/Li$_2$O formation (eqn-3).
**Fig. S1** PXRD patterns of MFor [M = Zn (FOR1), Co (FOR3) and ZnCo (FOR4)] with their simulated PXRD pattern.

**Fig S2** Ex-situ PXRD patterns of the electrodes of bare FOR1, and those b) discharged to 0.005 V, c) charged to 3.0 V and d) after 60 cycles. Lines due to Cu-current collector are marked with *.
Fig.S3 FESEM images of the FOR1 \([\text{Zn}_3(\text{HCOO})_6]\) plates at two different magnifications

Fig. S4 TEM images of the diamondoid FOR1 \([\text{Zn}_3(\text{HCOO})_6]\) at two different magnifications
Fig. S5  Galvanostatic charge–discharge cycle curves for FOR2 (a) 1st cycle and (b) selected cycles. (Current density of 60 mA/g (0.11C) plot. Potential window 0.005 – 3 V, recorded at room temperature)

Figure S6 PXRD patterns of FOR1, FOR3 and FOR4
FTIR of ZnO

CAS Registry Number: 1314-13-2
Formula: ZnO
CA Index Name: Zinc oxide (ZnO)
SpectrumID: NIDA69905
Spectrometer: Nicolet 170SX or JASCO FT/IR-410

Source: Integrated Spectral Database System of Organic Compounds. (Data were obtained from the National Institute of Advanced Industrial Science and Technology (Japan))