## **Supporting Information for**

# Nickel salicylaldoxime based coordination polymer as a cathode for lithiumion batteries

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## 1. Material characterisation data

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Figure S2. FTIR spectra of II, KBr

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Figure S3. FTIR spectra of III, KBr

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Figure S4. FTIR spectra of IV, KBr



Figure S6. Powder XRD diffraction patterns of samples I-IV



Figure S7. TGA curve of sample IV

#### Quantum chemical data

The metal center in the reported MOPs is similar to that in NiSalen; however, the bridging fragment is significantly different, since the ligands in the adjacent units of the polymer chain can form two (N)O–H···O(C) hydrogen bonds with each other (Fig.S8). Unlike the N–C<sub>2</sub>H<sub>4</sub>–N bridge in Salen, the combination of two hydrogen bonds offers far superior structural flexibility, allowing for a more planar structure of MOP, as compared to NiSalen and similar complexes. Furthermore, in contrast to [NiSalEn]<sub>n</sub> oligomers, which form twisted structures upon oxidation due to rotation around C–C bonds between the aromatic rings, DFT calculations for model MOPs do not demonstrate appreciable deviations from planarity upon stepwise removal of electrons, which is attributed to the rigidity of both the coordination site and the ligand itself.



Figure S8. Optimized geometries of (a) [NiL<sub>2</sub>]<sup>2-</sup> and (b) [Ni<sub>3</sub>L<sub>3</sub>]<sup>0</sup>, DFT calculations

Despite the inherent inequality of peripheral and inner structural units in short-oligomer models of MOP, the results of DFT calculations can still be used to elucidate the possible electronic structure changes in course of the oxidation process. Available computational data suggests that oxidation of MOPs is predominantly ligand-centered, and the involvement of the metal atoms is small.



**Figure S9.** Charge distribution in the [Ni<sub>3</sub>L<sub>3</sub>]<sup>0</sup> during the stepwise oxidation, DFT calculations