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## Electronic supplementary information (ESI) for

## The effect of Nitrogen and Oxygen Coordination: Toward a

## Stable Anode for Reversible Lithium Storage

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Fig. S1 The local structure of Co-pydc with abundant water coordinated in its channels.



Fig. S2 SEM micrographs of evacuated Co-pydc (a, and c) and Co-BDC (b, and d) at different magnification.



**Fig. S3** Nitrogen adsorption/desorption isotherms and pore-size distribution of evaluated Cobiding (a, c) and Co-BDC (b, d).



**Fig. S4** (a) Rate performance of the evacuated Co-pydc at different current densities ranging from 100 to 2000 mA  $g^{-1}$ . (b) The corresponding charge-discharge profiles of the rate test.



Fig. S5 Probable lithiation sites of of (a) evacuated Co-pydc and (b)Co-BDC.

The Co<sup>2+</sup> ions in evacuated Co-pydc are segregated by organic linkers and not fully coordinated for the remove of water. We anticipate that more Li ions will be captured by the organic linkers, especially by the uncoordinated carboxy groups and the Co(0) generated at discharged state would not aggregate with each other. While for Co-BDC, the Co<sup>2+</sup> ions are all hesacoordinated by oxygen atoms and the CoO<sub>6</sub> octahedral are connected with each other to form inorganic metal-oxide layers. Thus, more Li ions will be intercalated to the metal-oxide layers and the metals are more likely to aggregate with each other during the repeated cycles.



Fig. S6 XRD patterns of evacuated Co-pydc and Co-BDC electrode before and after one cycle.



**Fig. S7** SEM micrographs of evacuated Co-pydc electrode before and after one cycle (a, and c) and Co-BDC electrode before and after one cycle (b, and d) at the same magnification.