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Two isomorphous coordination polymers derived metal oxides as high performance anodes for lithium-ion batteries

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Thermal analyses of compounds **1** and **2** were performed in the temperature range of 30-800 °C on a NETZSCH STA 449F3 analyzer in air with an increasing temperature rate of 10 °C/min.



Fig. 1S TGA analysis of (a) compound 1 and (b) compound 2

Nitrogen adsorption-desorption isotherms were obtained from the N₂ physisorption at 77K using 3H-2000PS1 nitrogen adsorption apparatus. The Brunauer-Emmett-Teller (BET) specific surface areas (S_{BET}) were calculated using the BET equation, and the pore size were calculated by desorption isotherm using the Barret-Joyner-Halender (BJH) method. And it can be calculated that the BET specific surface area are 16.1 m²/g and 7.3 m²/g. The pore size distribution (PSD) plots calculated from the desorption branches of the nitrogen sorption isotherms. According to the PSD curves, the cumulative pore volume of the compounds **1** and **2** are 0.1 ml/g and 0.07 ml/g, the average pore diameter are 17.3 nm and 16.9 nm, respectively.



Fig. 25 Nitrogen adsorption-desorption isotherms and corresponding pore size distribution curves of the (a) compound 1 and (b) compound 2

It can be calculated that the BET specific surface area are $3.7 \text{ m}^2/\text{g}$ and $9.8 \text{ m}^2/\text{g}$ of Co_3O_4 and NiO. The pore size distribution (PSD) plots calculated from the desorption branches of the nitrogen sorption isotherms. According to the PSD curves, the cumulative pore volume of Co_3O_4 and NiO are 0.15 ml/g and 0.19 ml/g, the average pore diameter are 51.2 nm and 21.3 nm, respectively.



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Fig. 3S Nitrogen adsorption-desorption isotherms and corresponding pore size distribution curves of the (a) Co₃O₄ and (b) NiO



Fig. 4S Electrochemical impedance spectra (EIS) of the (a) Co₃O₄ electrode and (b) NiO electrode at 2000 mA/g after different cycles

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Table 15 Selected bond distances (A) an	d angles (deg) for compound 1.		
Co(1)-N(1)	2.1128(18)	Co(1)-N(1) ^{#1}	2.1129(18)
Co(1)-O(2) ^{#2}	2.1084(15)	Co(1)-O(1) ^{#3}	2.1964(15)
O(2) ^{#2} -Co(1)-N(1)	94.19(7)	N(1) ^{#1} -Co(1)-O(1) ^{#3}	93.99(7)
O(2) ^{#3} -Co(1)-N(1)	102.70(7)	O(2) ^{#2} -Co(1)-O(1) ^{#3}	101.06(6)
O(2) ^{#2} -Co(1)-O(1) ^{#2}	61.19(6)	N(1)-Co(1)-N(1)#1	87.68(10)

Table **1S** Selected bond distances (Å) and angles (deg) for compound **1.**

* Symmetry mode: #1 -x+1,y,-z+3/2; #2 -x+3/2,y+1/2,-z+3/2; #3 x-1/2,y+1/2,z