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Single crystal polyoxoniobate as a precursor to form uniformly distributed NbO/Cu nanocrystalline@N-doped carbon loaded onto reduced graphene oxide for high rate and high capacity Li/Na Storage

Peng Huang,[‡a] Min Huang,[‡a] Hai Hu,[a] Yuan Zhong,[a] Chao Lai,[a] and Shulei Chou*[b]

[a.] Jiangsu Key Laboratory of Green Synthetic Chemistry for Functional Materials, Department of Chemistry, School of Chemistry and Material Science, Jiangsu Normal University, Xuzhou, 221116, PR China.

[b.] Institute for Superconducting and Electronic Materials, University of Wollongong, Squires Way, North Wollongong, NSW 2500, Australia. E-mail: shulei@uow.edu.au.

Results and Discussion

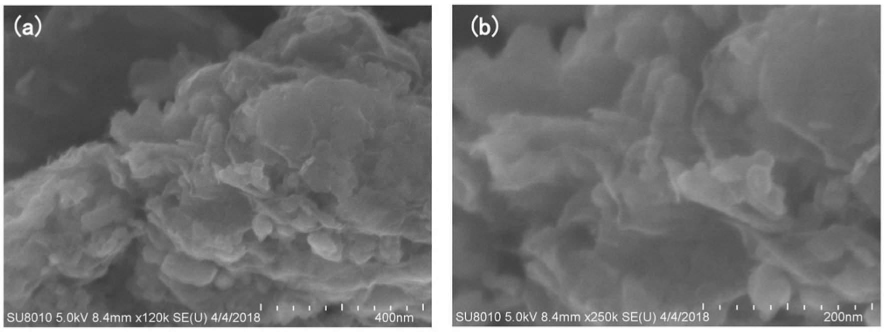

Figure S1. SEM image of NbO/Cu@NC-RGO.

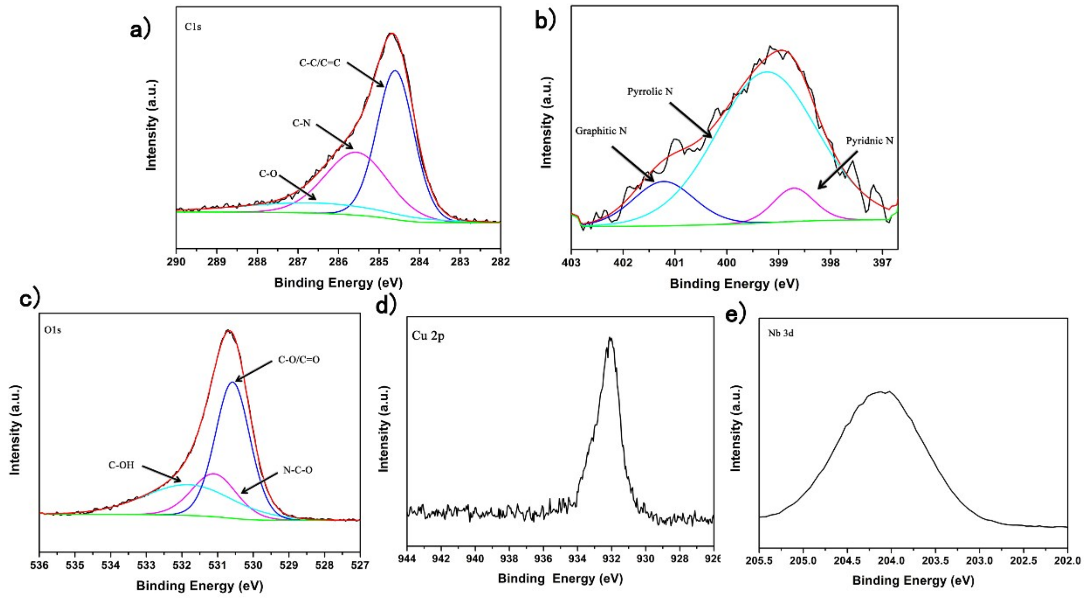

Figure S2. High resolution XPS spectra of (a) C 1s, (b) N, (c) O1s, (d) Cu 2p, and (e) Nb 3d of NbO/Cu@NC-RGO, respectively.

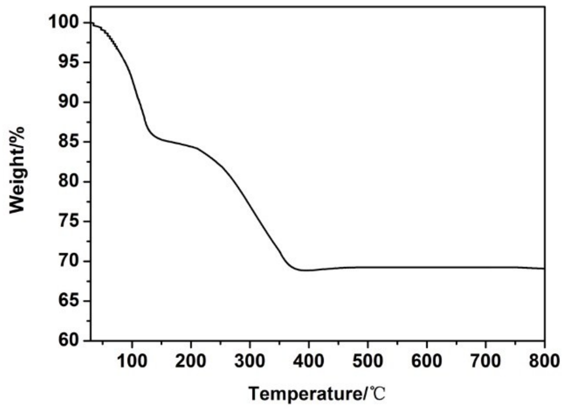

Figure S3. The TG curve of $K_5[Cu(en)_2]_{15.5}[(Nb_{24}O_{72}H_6)_2]\cdot 94.5H_2O$. $K_5[Cu(en)_2]_{15.5}[(Nb_{24}O_{72}H_6)_2]\cdot 94.5H_2O$ exhibits two weight loss steps in the temperature range 30-800 °C, the first weight loss is 15.17% (theoretical value 14.76%) in the temperature range 30-200°C, corresponding to the loss of noncoordinated and coordinated water molecules. And the second weight loss is 17.32 % in the temperature range 200-400°C, corresponding to the loss of ethanediamine molecules, which is consistent with the theoretical value 16.17%.

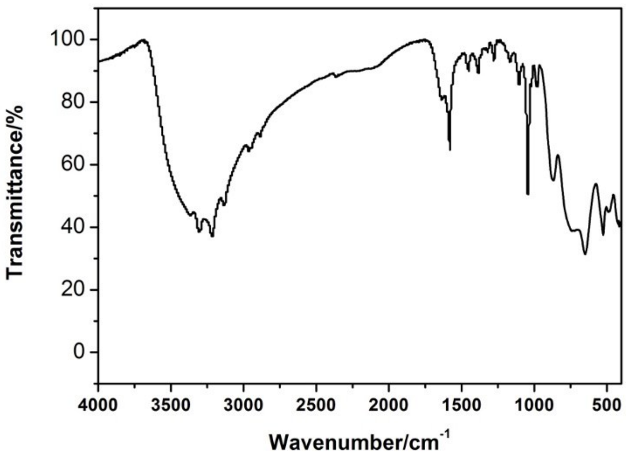

Figure S4. The IR spectrum of $K_5[Cu(en)_2]_{15.5}[(Nb_{24}O_{72}H_6)_2]\cdot 94.5H_2O$. The characteristic peaks at 1110, 1040, 975, 874, 650 and 526 cm^{-1} are assigned to the ν(Nb–O_t) and ν(Nb–O–Nb) stretches. The ν(Nb–Ob–Nb)vibration frequencies in the region 500–900 cm^{-1} show evident red shifts compared with those of the precursor $K_7HNb_6O_{19}\cdot 13H_2O$, suggesting that the Cu–O interactions between Cu and O of polyoxoniobate.

Table S1. Comparison the electrochemical performance of our samples with other niobium oxide anode materials for lithium-ion batteries.

Sample	Capacity (mAh g^{-1})	Rate capability	Ref.
NbO/Cu@NC-RGO	580 mAh g^{-1} at 0.1 A g^{-1}	342 mAh g^{-1} at 0.5 A g^{-1}	This work
NbO-BM	380 mAh g^{-1} at 0.1C	216 mAh g^{-1} at 0.5C	1
NbO	293 mAh g^{-1} at 0.1C	162 mAh g^{-1} at 0.5C	1
Nb_2O_5 Nanosheets	184 mAh g^{-1} at 0.2 A g^{-1}	90 mAh g^{-1} at 1 A g^{-1}	2
Nb_2O_5 Nanoparticles	145 mAh g^{-1} at 0.5 A g^{-1}	120 mAh g^{-1} at 1 A g^{-1}	3
T-Nb_2O_5/Graphene	145 mAh g^{-1} at 0.5 A g^{-1}	115 mAh g^{-1} at 2 A g^{-1}	4
Ag-1D T-Nb_2O_5	179 mAh g^{-1} at 0.5 A g^{-1}	103.6 mAh g^{-1} at 5 A g^{-1}	5
Bulk $Ti_2Nb_{10}O_{29}$	238 mAh g^{-1} at 0.792 A g^{-1}	168 mAh g^{-1} at 3.96 A g^{-1}	6
$Ti_2Nb_{10}O_{29}$/rGo	261 mAh g^{-1} at 0.03 A g^{-1}	165 mAh g^{-1} at 0.5 A g^{-1}	7
Porous $Li_4Ti_5O_{12}$	168.1 mAh g^{-1} at 0.2 C	116 mAh g^{-1} at 20 C	8

Table S2. Comparison the electrochemical performance of our samples with other niobium oxide anode materials for sodium-ion batteries.

Sample	Capacity (mAh g^{-1})	Rate capability	Ref.
NbO/Cu@NC-RGO	203 mAh g^{-1} at 0.05 A g^{-1}	119 mAh g^{-1} at 0.8 A g^{-1}	This work
Porous Nb_2O_5 film	185 mAh g^{-1} at 0.1 A g^{-1}	84 mAh g^{-1} at 2 A g^{-1}	9
Nb_2O_5 nanosheet	145 mAh g^{-1} at 0.05 A g^{-1}	47 mAh g^{-1} at 1 A g^{-1}	10
Porous Nb_2O_5/C	180 mAh g^{-1} at 0.05 A g^{-1}	71 mAh g−1 at 1 A g−1	11
Nb_2O_5/Graphene	220 mAh g^{-1} at 0.05 A g^{-1}	102 mAh g^{-1} at 2 A g^{-1}	12
T-Nb_2O_5/CNFs	150 mAh g^{-1} at 1 A g^{-1}	97 mAh g^{-1} at 8 A g^{-1}	13
Nb_2O_5@C/rGO-50	120 mAh g^{-1} at 1.25 A g^{-1}	109 mA h g^{-1} at 3 A g^{-1}	14

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