Electronic Supplementary Information

Rational designing of $NiMoO_4$/carbon nanocomposites for high-performance supercapacitors: an *in situ* carbon incorporation approach

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1. The calculation for the compositions of $NiMoO_4$ and carbon components in $NiMoO_4$/C (D50) nanocomposite using TGA curves:

At 600 °C:

Wt. retention percentage (x%) of $NiMoO_4$ = 97.4%
Wt. retention percentage (y%) of CNS = 0.9%
Wt. retention percentage (composite%) of $NiMoO_4$/C (D50) = 69.5%

Assume, the proportion of $NiMoO_4$ and carbon components in the nanocomposite as 'a' and 'b', respectively.

$$a + b = 1 \quad (1)$$

$$x\% \times a + y\% \times b = \text{composite}\ \% \times 1$$

$$\left(\frac{97.4}{100} \times a\right) + \left(\frac{0.9}{100} \times b\right) = \left(\frac{69.5}{100} \times 1\right)$$

$$0.974a + 0.009b = 0.695 \quad (2)$$

Equation (2) is divided by 0.009

$$\frac{0.974a}{0.009} + \frac{0.009b}{0.009} = \frac{0.695}{0.009}$$

$$108.222\ a + b = 77.22 \quad (3)$$

Subtract equation (1) from equation (3), and simplify

$$107.222a + 0 = 76.2$$

$$a = \frac{76.22}{107.222}$$

$$a = 0.711$$

a = 71.1% of $NiMoO_4$ and b = 28.9% of carbon components.

Therefore, 71.1% of $NiMoO_4$ and 28.9% of carbon components are calculated to be in $NiMoO_4$/C (D50) nanocomposite.

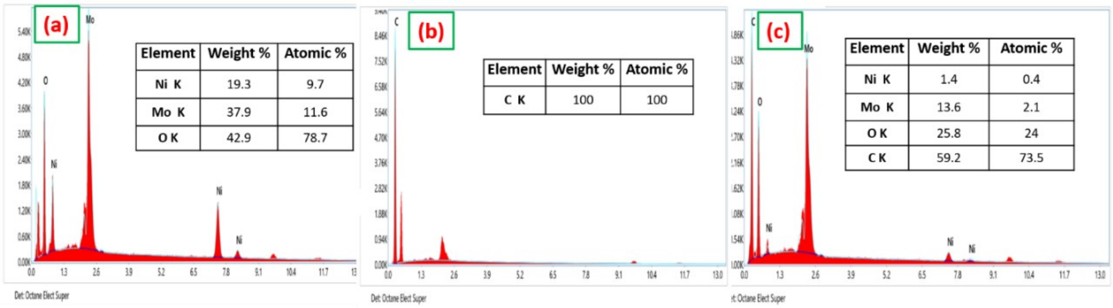

Fig. S1 EDAX analysis of elements present in the samples: (a) $NiMoO_4$, (b) CNS and (c) $NiMoO_4$/C (D50).

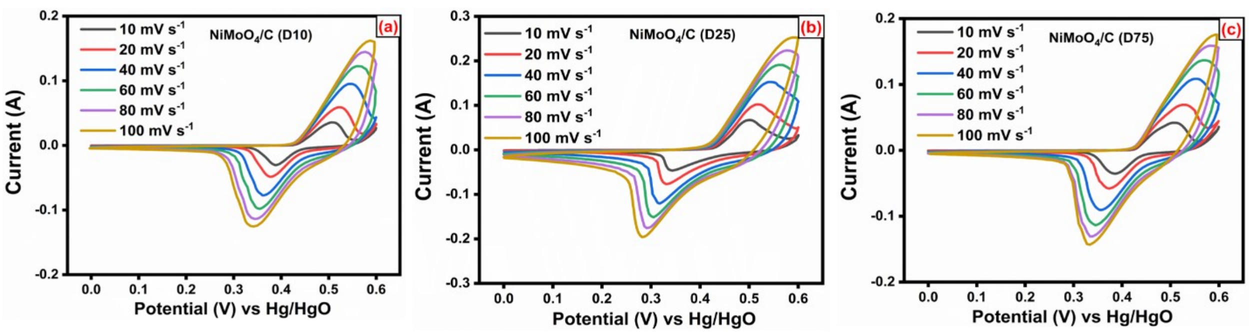

Fig. S2 CV curves of (a) $NiMoO_4$/C (D10), (b) $NiMoO_4$/C (D25) and (c) $NiMoO_4$/C (D75) at different scan rates (10–100 mV s^{-1}).

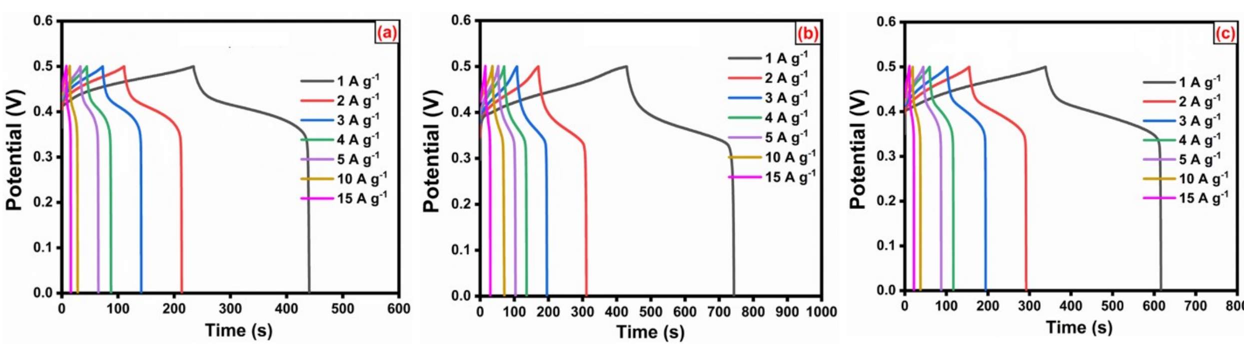

Fig. S3 GCD curves at different current densities (1–15 A g^{-1}): (a) $NiMoO_4$/C (D10), (b) $NiMoO_4$/C (D25) and (c) $NiMoO_4$/C (D75).

Table S1. Three electrode specific capacitance of $NiMoO_4$, CNS and $NiMoO_4$/C based nanocomposites at current density of 1 A g^{-1} using 3 M KOH as electrolyte.

S. No.	Electrode Materials	Specific capacitance (F g^{-1})
1	$NiMoO_4$	520
2	CNS	75
3	$NiMoO_4$/C (D10)	436
4	$NiMoO_4$/C (D25)	583
5	**$NiMoO_4$/C (D50)**	**940**
6	$NiMoO_4$/C (D75)	508

Table: S2 Electrical parameters of $NiMoO_4$, CNS, and $NiMoO_4$/C (D50) electrode materials estimated using ZSimpWin circuit fitting software for EIS experimental data.

Electrode materials	**R_s (Ω.cm²)**	**R_{pore} (mΩ. cm²)**	**R_{CT} (Ω.cm²)**	**Q_c (S.cm⁻². sⁿ)**	**n**	**Q_{dl} (S.cm⁻². sⁿ)**	**n**	**W (S.cm⁻². s^0.5)**	**χ^2**
$NiMoO_4$	1.15	0.95	13.02	0.0032	0.78	0.0229	0.32	4.091×10^{-12}	0.0032
CNS	1.07	57.7	5.58×10^{-5}	0.0012	0.70	0.0005	0.90	1.034×10^{-4}	0.0007
$NiMoO_4$/C (D50)	1.16	5.48	2.96	0.0024	0.82	0.0236	0.34	6.465×10^{-12}	0.0033

R_s - solution resistance, R_{pore} - coating pore resistance, R_{ct} - charge transfer resistance, CPE - constant phase element, n - exponent of CPE, W -Warburg impedance and χ^2 - chi-square value.

Table S3 Comparison of the present work with previously reported $NiMoO_4$-based nanomaterials.

S. No.	Electrode Materials	Method	Specific capacitance ($F\ g^{-1}$)	Cyclic stability (capacity retention % at no. of cycles)	Ref.
1	Mn-doped $NiMoO_4$/rGO	Solvothermal	689	96% at 200 cycles	1
2	$NiMoO_4$/rGO nanocomposite	Hydrothermal	1400	91% at 2000 cycles	2
3	Hierarchical carbon sphere @$NiMoO_4$	Two-step hydrothermal	268	88% at 2000 cycles	3
4	$NiMoO_4$/C Composite	Hydrothermal	325	56% at 10000 cycles	4
5	$NiMoO_4$/carbon composites	Solvothermal	805	92% at 6000 cycles	5
6	g-C_3N_4/$NiMoO_4$	Chemical precipitation	398	70% at 4000 cycles	6
7	$NiMoO_4$/reduced graphene oxide composite	Hydrothermal method	680	68% at 4000 cycles	7
8	$NiMoO_4$ nanorods and hierarchical nanospheres	Facile hydrothermal	974	91% at 5000 cycles	8
9	Carbon nanofibers/$NiMoO_4$ nanoparticles	Electrospinning	1438	92% at 3000 cycles	9
10	Ni-doped $MnMoO_4$	One-step hydrothermal method	2315	96 % at 5000 cycles	10
11	$NiMoO_4$/rGO nanocomposite	Hydrothermal method	1516	96% at 10000 cycles	11
12	$NiCo_2S_4$/$NiMoO_4$	Hydrothermal method	2323	90% at 10000 cycles	12
13	$NiMoO_4$@$CoMoO_4$	Hydrothermal method	1282	76% at 1000 cycles	13
14	**$NiMoO_4$/C (D50)**	***In situ* Hydrothermal carbonization**	**940**	**71% at 5000 cycles**	***This report***

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