Supporting information

In-situ growth of $NiSe_2$ nanoparticles on g-C_3N_4 nanosheets for efficient hydrogen evolution reaction

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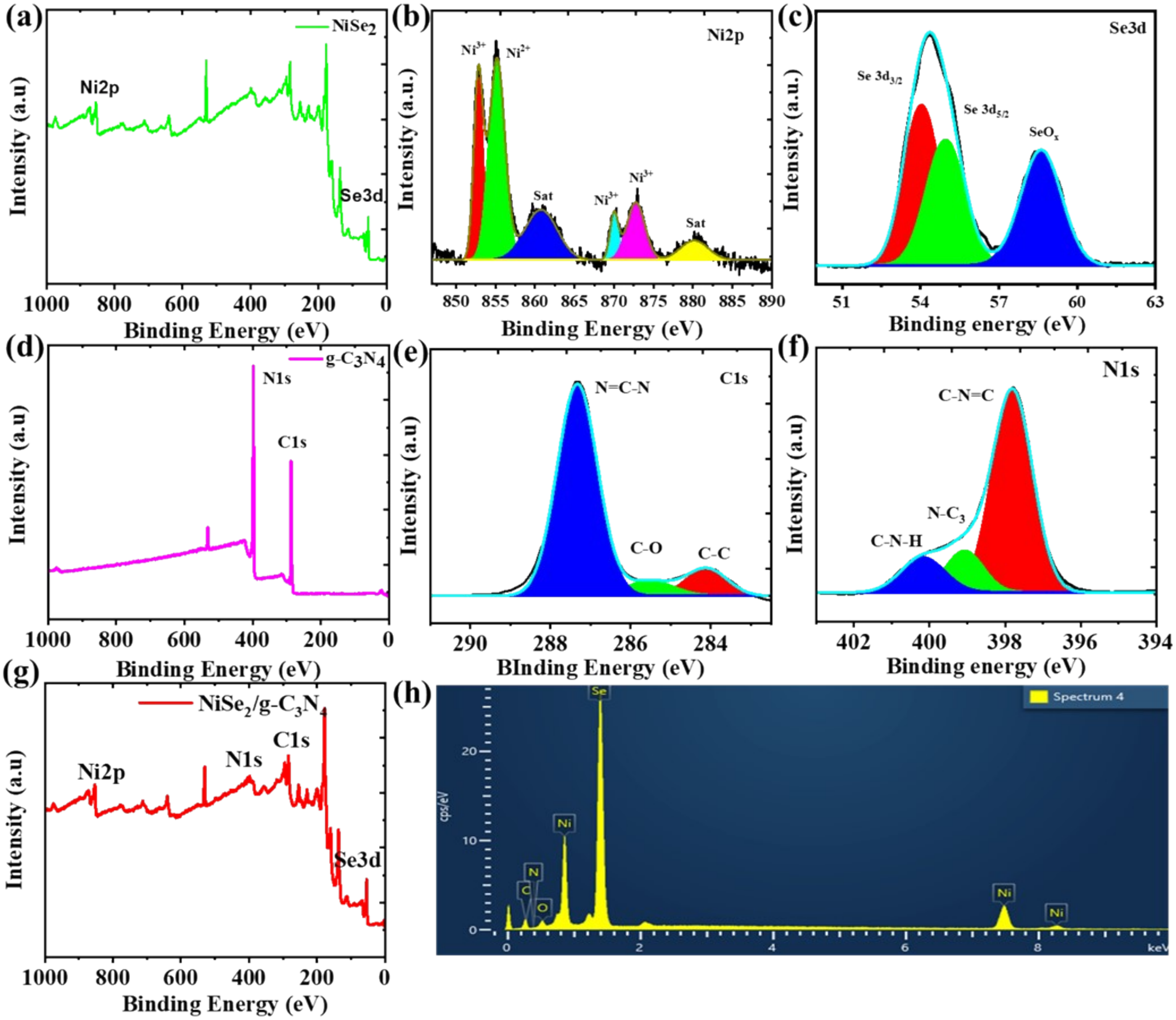

Fig. S1. *XPS survey spectra of* ***(a)*** *$NiSe_2$ and XPS high resolution spectra of* ***(b)*** *Ni2p, and* ***(c)*** *Se3d of bare $NiSe_2$. XPS survey spectra of* ***(d)*** *g-C_3N_4 and XPS high resolution spectra of* ***(e)*** *C1s and* ***(f)*** *N1s. XPS survey spectra of* ***(g)*** *$NiSe_2$/ g-C_3N_4.* ***(h)*** *Energy dispersive spectroscopy (EDS) spectrum of $NiSe_2$/g-C_3N_4.*

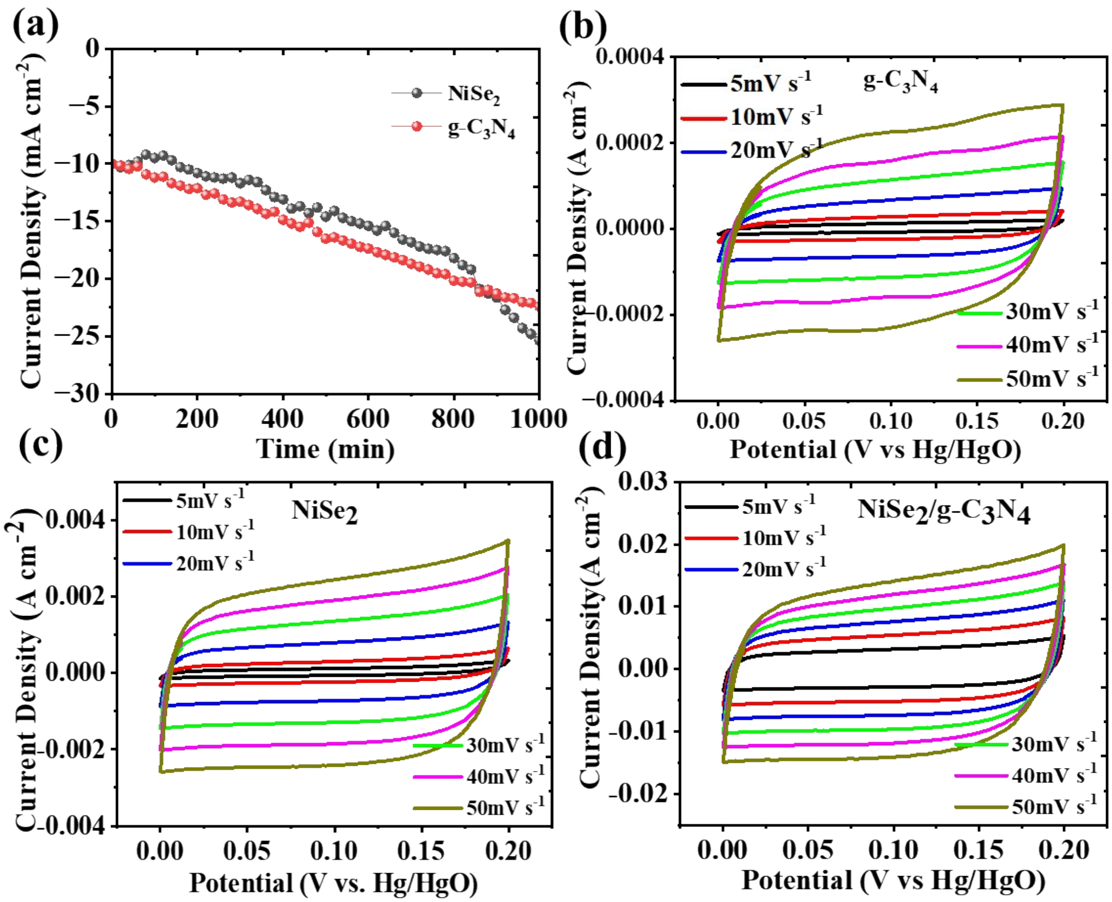

Fig. S2. (a) Time dependence of current density under static potentialfor $NiSe_2$ and g-C_3N_4 respectively ***(b-d)*** *CV curves of g-C_3N_4, $NiSe_2$, and $NiSe_2$/g-C_3N_4, electrodes in 1 M KOH.*

Table S1. The electroactivity comparison of various catalysts towards HER (measured at current density 10 mA cm^{-2})

Sample	Electrolyte	Overpotential (mV)	Tafel Slope (mV dec^{-1})	Ref.
$NiSe_2$	0.5 M H_2SO_4	198	72.1	1
NiSe NWs	1.0 M KOH	96	120	2
$NiSe_2$ NCs	0.5 M H_2SO_4	190	44	3
$NiSe_2$/NFs	1.0 M KOH	252	59.3	4
$NiSe_2$@NG	0.5 M H_2SO_4	163	74.2	5
$NiSe_2$/CNT	0.5 M H_2SO_4	159	35.6	6
$NiSe_2$-T@NC	0.5 M H_2SO_4	196	45	7
F/P-$NiSe_2$/CC	1.0 M KOH	53	95.6	8
$Ni_{0.8}Fe_{0.2}Se_2$	0.5 M H_2SO_4	64	43	9
$NiSe_2$@Ru	1.0 M KOH	136	48.7	10
$NiSe_2/MoS_2$	0.5 M H_2SO_4	143	45	11
$MoS_2/NiSe_2$/rGO	1.0 M KOH	152	73	12
$NiSe_2/Ti_3C_2T_x$	0.5 M H_2SO_4	200	37.7	13
$NiSe_2$-NPs/CNTs/Ni-MOF NS	1.0 M KOH	95	82	14
$NiSe_2/MoSe_2$	0.5 M H_2SO_4	147	43.5	15
$MoSe_2/SnS_2$	1.0 M KOH	285	109	16
$CoSe_2$/rGO/MWCNT	0.5 M H_2SO_4	125	52	17
MXene-F,N-gCW-$CoSe_2$	1 M KOH	116.8	84.2	18
$NiSe_2$/g-C_3N_4	**1 M KOH**	**87**	**64**	**This work**

Calculation

1) The Fowkes approach:

To calculate the surface free energy of the substrate, three or more liquids with known surface tension parameters (polar and dispersion components) must be used. To limit the potential of inaccuracy, it is recommended to use more liquids.

The equation to calculate surface free energy using the Fowkes approximation is as follows:

$$\left[\frac{1 + Cos\theta}{2}\right] \times \left[\frac{\gamma_l}{\sqrt{\gamma_l^d}}\right] = \sqrt{\gamma_s^p} \times \sqrt{\frac{\gamma_l^p}{\gamma_l^d}} + \sqrt{\gamma_s^d} \quad \textbf{(S1)}$$

The equation is of the form

$$Y(LHS) = mX\ (RHS) + C \quad \textbf{(S2)}$$

Where LHS can be derived by measuring for the liquids utilised. The values of γ_l and γ_l^d can be found in the standard table of surface tension parameters. Similarly, RHS can be determined using the polar and dispersion components of liquids. Plotting LHS vs. RHS yields a straight line with the intercept on the Y-axis. The slope and intercept are squared and combined to yield the total surface energy [19].

2) ECSA calculation:

The double layer capacitance (Cdl) can be calculated from a cyclic voltammetry (CV) experiment using the formula: Cdl= Δj (ja-jc)/2ν, where ja and jc represent the anodic and cathodic current densities respectively, measured at a potential difference ΔE = 0.1 V and ν denotes the scan rate in mVs^{-1}. The non-Faradic current density-based electrochemically active surface area (ECSA) can be estimated as: ECSA = Cdl/Cs, represents the specific capacitance of the electrode, taken as 0.04 $mFcm^{-2}$ in 1 M KOH electrolyte solution [20–23].

Sample Name	***C*dl**	**ECSA**
$NiSe_2$	10.9	275.5
g-C_3N_4	6.45	161.25
$NiSe_2$/g-C_3N_4	22.7	567.5

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