Supplementary material

NiO nanobelts exposed with {110} crystal planes as an efficient electrocatalyst for oxygen evolution reaction

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DFT Calculation For Oxygen Evolution Reaction (OER):

The atomic scale mechanisms of the OER are complicated and not fully established, insights into the thermodynamics of the reaction can be obtained using the scheme developed by Norskov et al [1]. In the scheme, the OER is assumed to involve four elementary reaction steps and each involves electron transfer of an electron to the electrode and a proton to water:

R1: $H_2O + * \longrightarrow *OH + H^+ + e^-$

R2: $*OH \longrightarrow *O + H^+ + e^-$

R3: $H_2O + *O \longrightarrow *OOH + H^+ + e^-$

R4: $*OOH \longrightarrow * + O_2 + H^+ + e^-$

Where * and *X denotes an adsorption site and an adsorbed X species, respectively; H_2O is a water molecule in liquid phase. Therefore, the free energy of the OER is computed by the formula $\Delta G = \Delta E + \Delta ZPE - T\Delta S$, where the ΔE can be obtained by the computation of geometrical structures. The value of ΔZPE and ΔS were determined by computed vibrational frequencies and standard table for the reactants and products in the gas phase and the entropy of adsorbed atoms or molecules at surface active site were set as zero. Moreover, for the total reaction $H_2O \longrightarrow {}^1/_2O_2 + H_2$, the free energy change was fixed at experiment value of 2.46 eV per water molecule. So the free energy change for reaction R1-R4 can be expressed as

$\Delta G_{R1} = \Delta G_{OH} - Ue$

$\Delta G_{R2} = \Delta G_O - \Delta G_{OH} - Ue$

$\Delta G_{R3} = \Delta G_{OOH} - \Delta G_O - Ue$

$\Delta G_{R4} = 4.92 - \Delta G_{OOH} - Ue$

Where U is the potential measured against normal hydrogen electrode at standard conditions.

The theoretical overpotential is defined as $\eta = \max\{\Delta G_{R1}, \Delta G_{R2}, \Delta G_{R3}, \Delta G_{R4}\}/e - 1.23\ (V)$.

Table S1. Details of the reaction conditions for the synthesis of NiO nanobelts and nanoplates

	Hydrothermal Reaction				Calcination
Morphology	NaOH (g)	$NiSO_4$ (g)	$Ni(NO_3)_2$ (g)	Temperature/Time (°C/h)	Temperature/Time (°C/h)
Nanobelts	0.1960	2.5759	-	120°C/4h	500°C/4h
Nanoplates	0.3000	-	2.9080	180°C/8h	300°C/2h

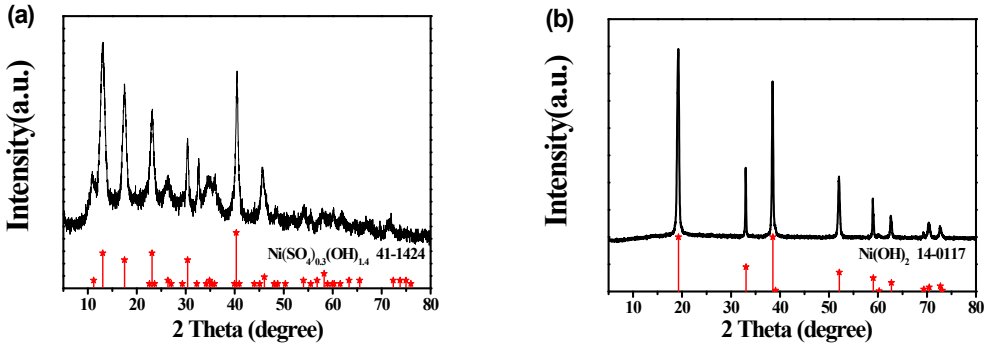

Fig. S1 XRD patterns of (a) nanobelts precursors and (b) nanoplates precursors.

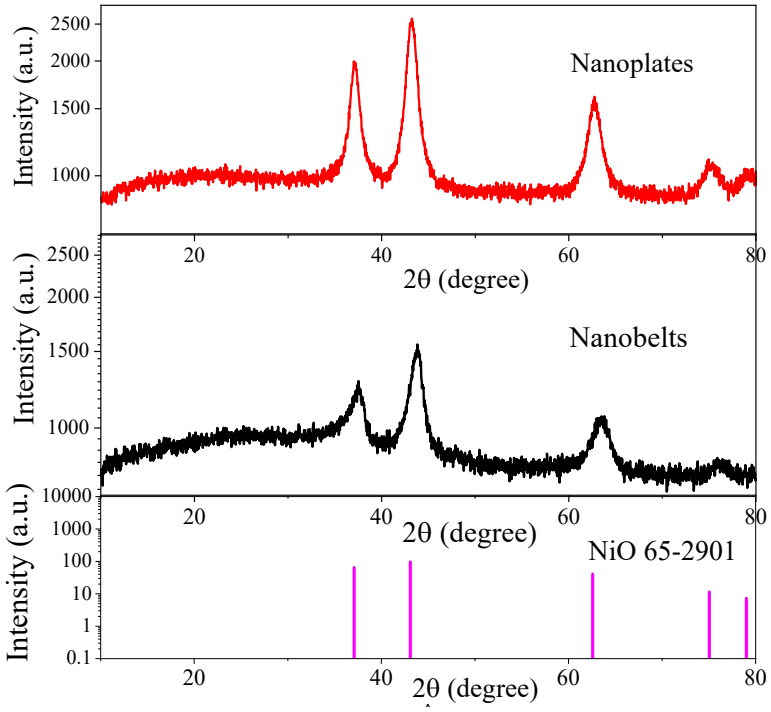

Fig. S2 XRD patterns of NiO nanobelts and nanoplates (Intensity was presented in logarithmic plot).

Table S2. Particle size, structural, surface area, porosity, and electrochemical performance of NiO nanobelts and nanoplates

Samples	Average crystallite size (nm)	Sizes of nanostructures	BET Surface area (m^2/g)	Total pore volume (mL/g)	Current density (mA/cm^2) at 400 mV overpotential	Tafel slope (mV/dec)	Specific capacitance (mF/cm^2)
Nanobelts	5.4	Length: 60 nm, Thickness: 20 nm	98.7	0.528	66.3	142.5	0.78
Nanoplates	5.5	Length: several micrometers, Width: 16 nm	153.0	0.183	15.4	154.2	3.6

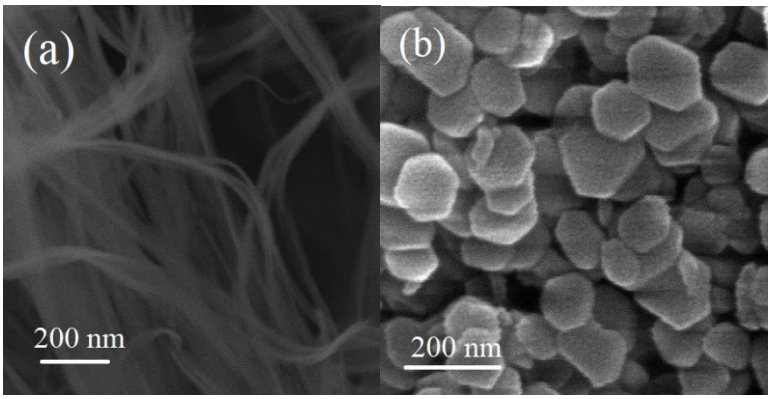

Fig. S3 SEM images of (a) NiO nanobelts precursors and (b) NiO nanoplates precursors.

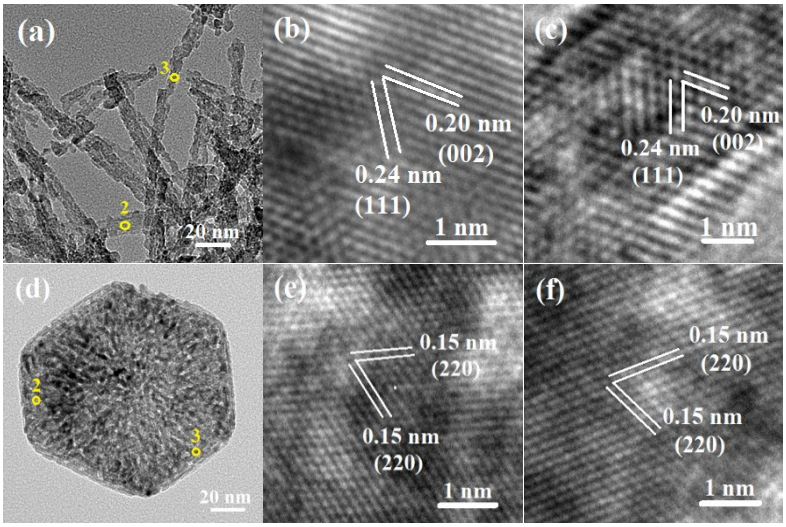

Fig. S4 (a-c) TEM and HRTEM images of NiO nanobelts at spot 2 and 3, (d-f) TEM and HRTEM images of NiO nanplates at spot 2 and 3,

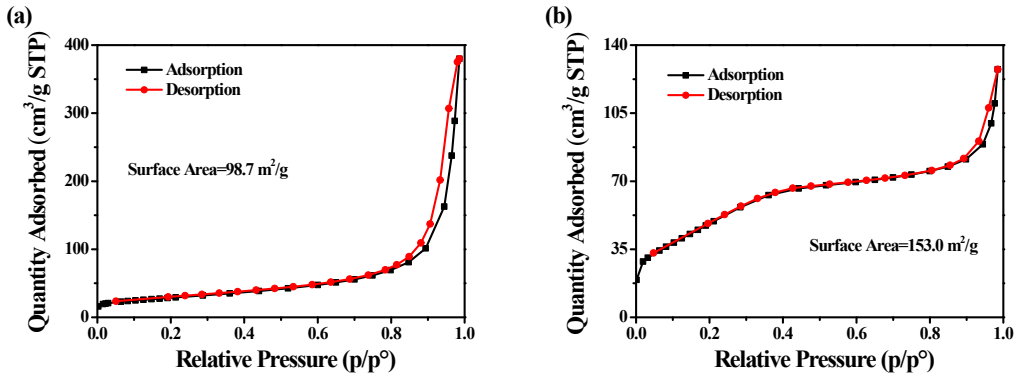

Fig. S5 Nitrogen absorption/desorption curves of (a) NiO nanobelts and (b) NiO nanoplates.

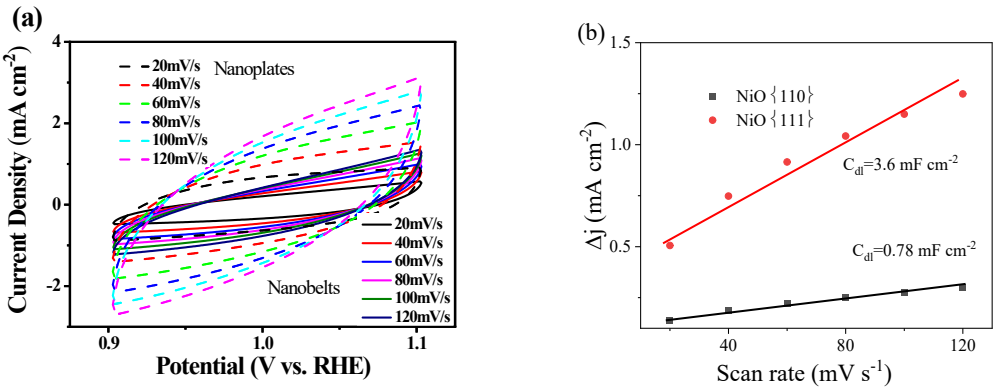

Fig. S6 (a) CV curves of NiO nanobelts and nanoplates at different scan rates, (b) Plots of capacitive currents with respect to scan rate normalized by active mass.

Table S3 OER performances comparison of reported representative Ni-based electrocatalysts

Catalysts	Current density ($mA\ cm^{-2}$)	Overpotential (mV)	Tafel slopes ($mV\ dec^{-1}$)	References
NiO/CeO_2 NW@CC	50	330	85	[2]
Mo–Ni/C	10	470	93	[3]
Ni @ NiO/N-C	10	390	100	[4]
N doped NiO	100	750	136	[5]
$NiCo_2O_4$/NiO-rGO	10	350	66	[6]
Ni@NiO Nanowires	10	382	103	[7]
NiO@C	100	500	92	[8]
NiO nanobelts	50	382	142.5	This work
	100	429		

References:

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