Supplementary Information

Hematite nanobelts with ordered oxygen vacancies for bifunctional electrocatalytic water splitting

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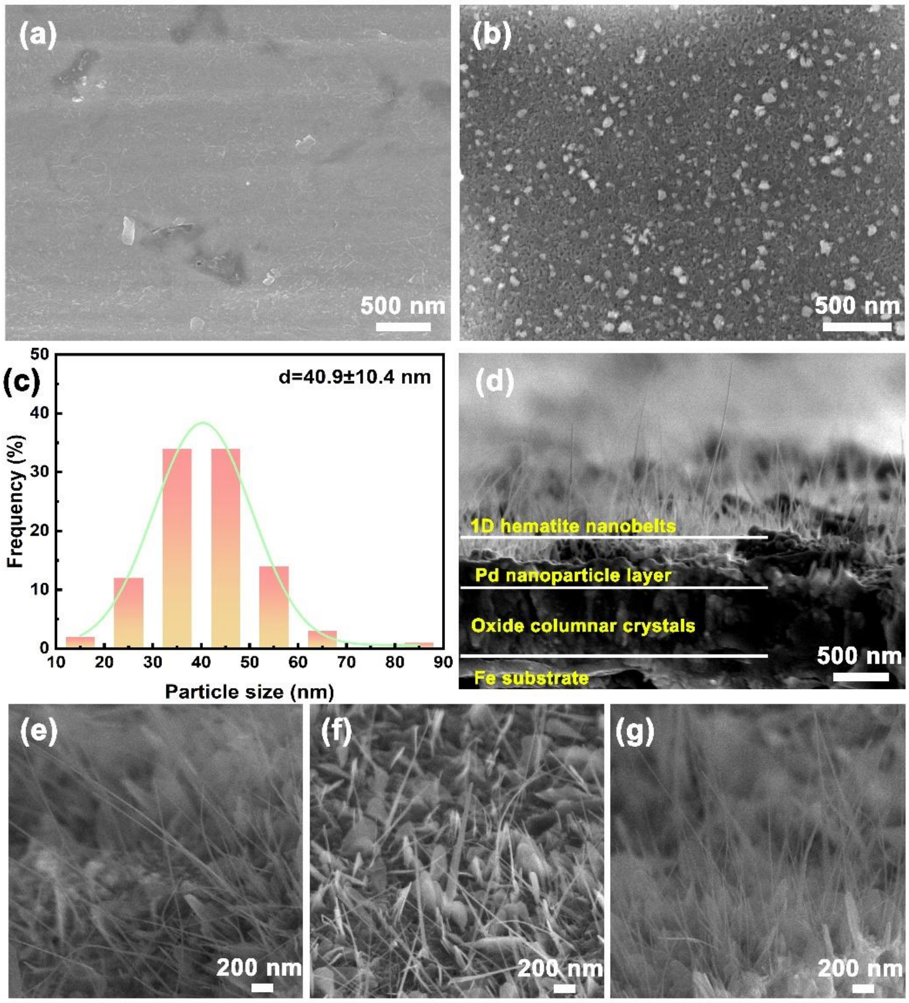

Figure S1. (a) SEM image of fresh iron foil after sandpaper treatment; (b) SEM image of Pd nanoparticles loaded on MgO pre-oxidized layer; (c) histogram of particle size distribution of Pd nanoparticles; (d) cross-sectional SEM image of HNBs-30; SEM frontal image of (e) HNBs, (f) HNBs-30 and (g) HNBs-60.

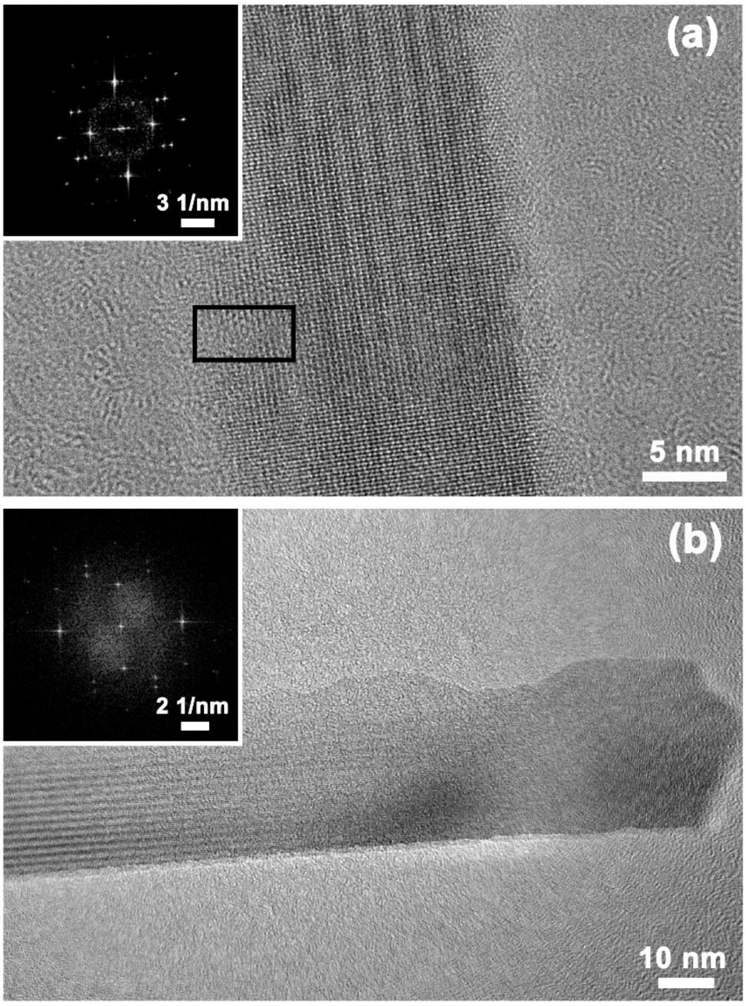

Figure S2. (a) HRTEM image of HNBs (The inset is a fast Fourier transform plot); (b) HRTEM image of HNBs-60 (The inset is a Fast Fourier Transform plot).

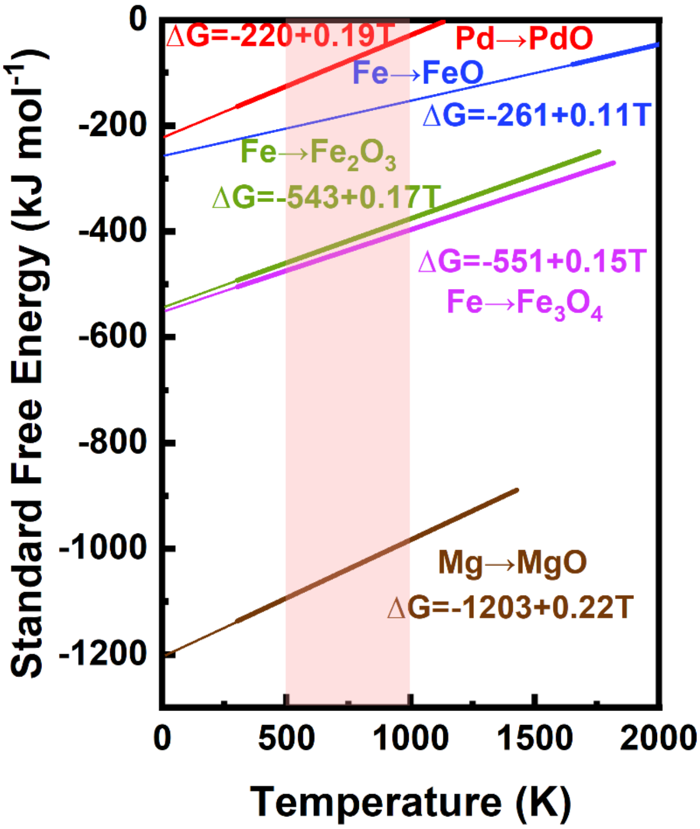

Figure S3. Ellingham diagram.

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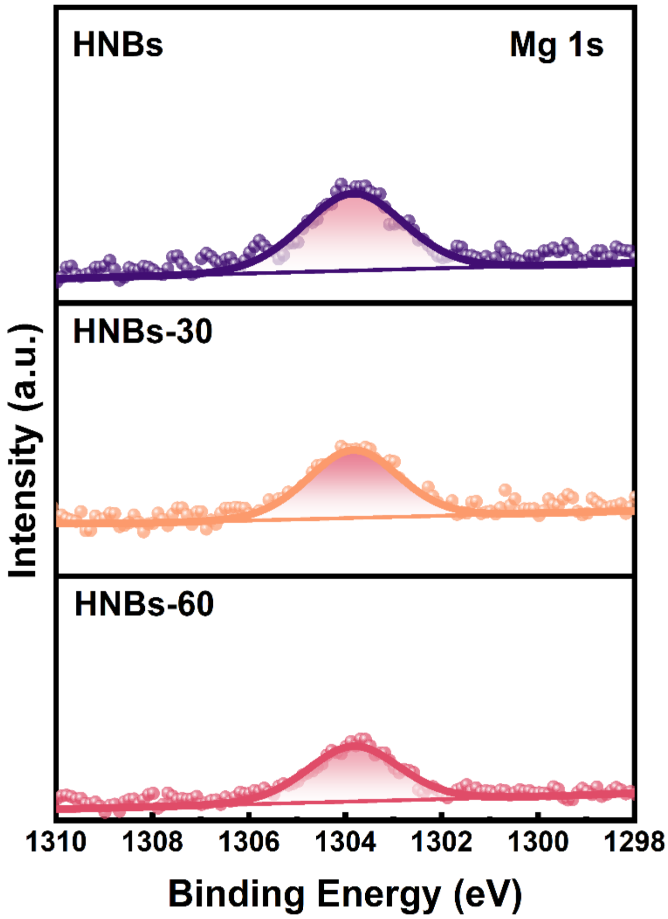

Figure S4. XPS high-resolution spectra of the Mg 1s region of HNBs, HNBs-30, and HNBs-60.

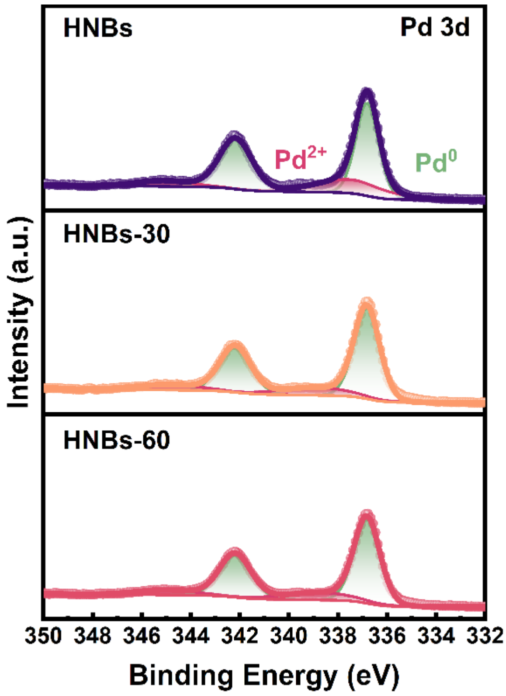

Figure S5. XPS high-resolution spectra of the Pd 3d region of HNBs, HNBs-30 and HNBs-60.

XPS high-resolution spectra of the Pd 3d region indicate the presence of surface Pd elements. Split-peak fitting according to the Pd^0 and Pd^{2+} orbitals resulted in electron binding energies of 336.6, 337.6, 342.2, and 345.1 eV for Pd^0 $3d_{5/2}$, Pd^{2+} $3d_{5/2}$, Pd^0 $3d_{3/2}$, and Pd^{2+} $3d_{3/2}$, respectively [S1]. Pd^0 $3d_{5/2}$ as well as Pd^0 $3d_{3/2}$ have an energy spacing of 5.6 eV. Indicating that Pd coexists as a large amount of Pd in the metallic state and a small portion of PdO, demonstrating the aforementioned growth mechanism of Pd-catalyzed oxygen reduction.

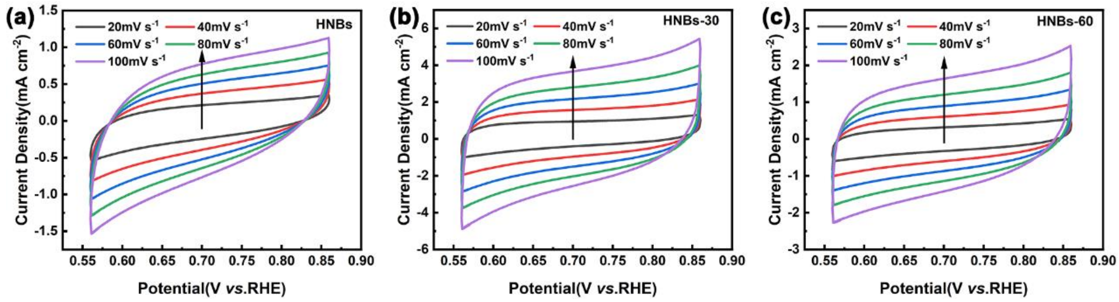

Figure S6. Scan rate dependence of the current densities in the CV curves of different HER catalysts with scan rates ranging from 20 mV s^{-1} to 100 mV s^{-1}. (a) HNBs, (b) HNBs-30, (c) HNBs-60.

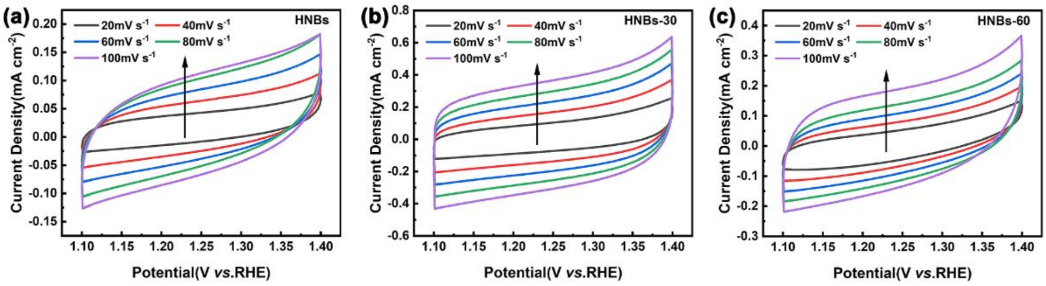

Figure S7. Scan rate dependence of the current densities in the CV curves of different OER catalysts with scan rates ranging from 20 mV s^{-1} to 100 mV s^{-1}. (a) HNBs, (b) HNBs-30, (c) HNBs-60.

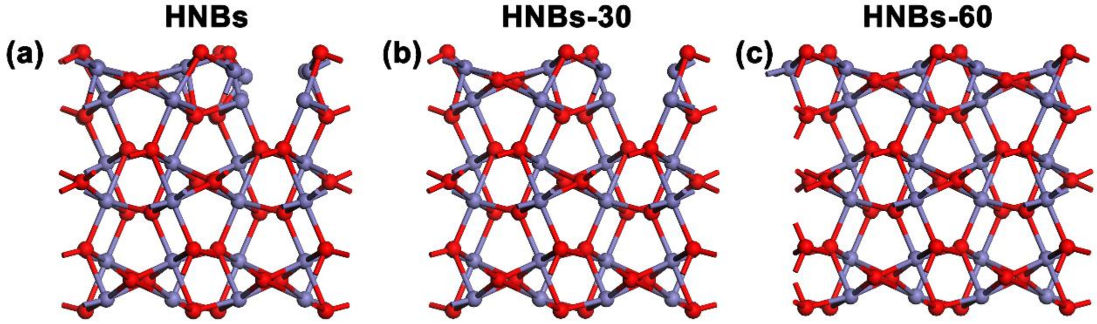

Figure S8. Structure models of (a) HNBs, (b) HNBs-30, and (c) HNBs-60 used for DFT calculation.

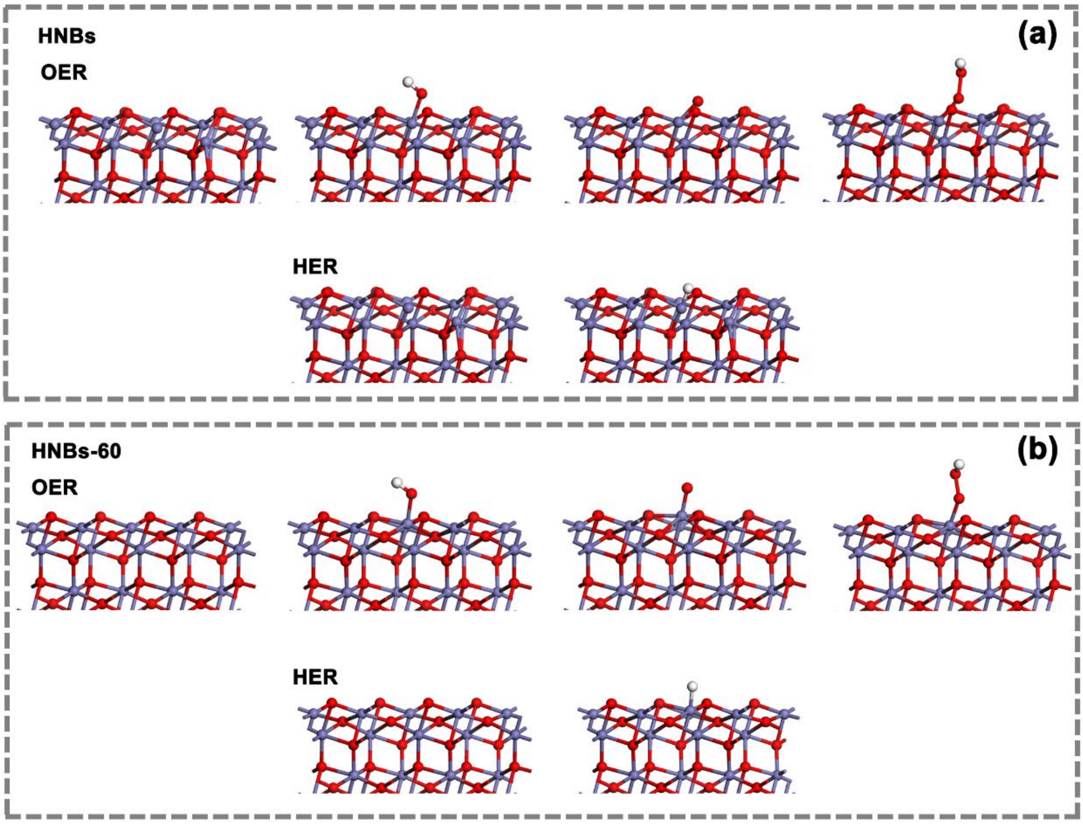

Figure S9. (a) Structure of the intermediates adsorbed on HNBs surface; (b) structure of the intermediates adsorbed on HNBs-60 surface.

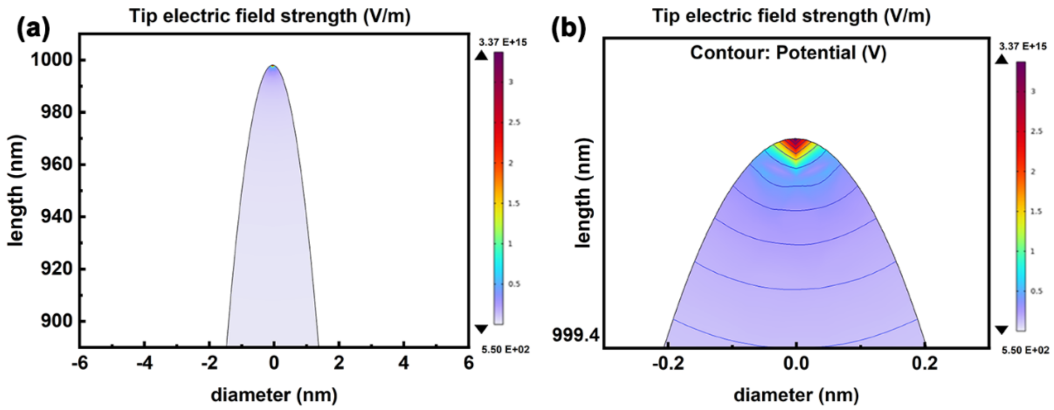

Figure S10. Calculation results from COMSOL. (a) distribution of the electric field strength of a single nanobelt under an applied positive potential; (b) distribution of the electric field strength at the tip.

Table S1. Peak areas of O 1s states in XPS spectra over the obtained samples.

Catalyst	O_L	O_V	O_S	$O_V/(O_L+O_V+O_S)$ %
HNBs	42050.51	51171.43	11585.32	48.82
HNBs-30	44944.33	45245.46	18648.23	41.57
HNBs-60	48704.24	30975.86	21315.68	30.67

Table S2. Fitting results of various resistances of hydrogen evolution system with different electrodes.

Catalyst	$R_s(\Omega)$	$R_{ct}(\Omega)$	$R_{int}(\Omega)$
HNBs	0.95	2.18	3.13
HNBs-30	1.04	1.16	2.20
HNBs-60	0.98	1.66	2.64

Table S3. HER overpotential and Tafel slope of HNBs-30 and other previously reported iron-based catalysts in this study.

Catalyst	J (mA cm^{-2})	Electrolyte	η (mV)	Tafel slope (mV dec^{-1})	iR correction	Ref.
Ni-Fe micro/nano urchin	10	1M KOH	124	114	NA	[S2]
SSFS	10	1M KOH	136	147	100%	[S3]
Fe-FVO-act	10	1M KOH	215	97.6	NA	[S4]
Mo-NiCo LDH(V_O)	10	1M KOH	194	94.5	90%	[S5]
Modified stainless steel	10	1M KOH	264	101	90%	[S6]
RuNiFe-O@SS	10	1M KOH	331	107	100%	[S7]
SS scrubber	10	1M KOH	373	121	NA	[S8]
This work	10	1M KOH	178	113	90%	/

Table S4. Fitting results of various resistances of oxygen evolution system with different electrodes.

Catalyst	$R_s(\Omega)$	$R_{ct}(\Omega)$	$R_{int}(\Omega)$
HNBs	1.30	4.58	5.88
HNBs-30	1.11	1.76	2.87
HNBs-60	1.28	2.87	4.15

Table S5. OER overpotential and Tafel slope of HNBs-30 and other previously reported iron-based catalysts in this study.

Catalyst	J (mA cm^{-2})	Electrolyte	η (mV)	Tafel slope (mV dec^{-1})	iR correction	Ref.
Vo-α-Fe_2O_3@AuNSs	10	1M KOH	282	87	NA	[S9]
NiFe-O@SS	10	1M KOH	391	73	100%	[S7]
Pt-α-Fe_2O_3/NF	10	1M KOH	304	49.6	90%	[S10]
SS scrubber	10	1M KOH	418	63	NA	[S8]
evo-FeOOH	10	1M KOH	350	40.6	95%	[S11]
α-Fe_2O_3 nano rods/CC	10	1M KOH	331	107	100%	[S12]
ε-Fe_2O_3	10	1M KOH	370	48	100%	[S13]
This work	10	1M KOH	317	44	90%	/

Table S6. Comparison of overall water splitting performance with of previous studies and this work in 1.0 M KOH solution.

Catalyst	J (mA cm^{-2})	Electrolyte	Cell voltage (V)	Ref.
Steel-3min	100	1M KOH	2.08*	[S14]
Fe-Ni_2P@PC/Cu_xS	100	1M KOH	2.10*	[S15]
$Co_1Fe_1Mo_{1.8}$ONMs@NF	100	1M KOH	2.23*	[S16]
SS-Scrubber-CA	100	1M KOH	2.25*	[S8]
PSD-SM	100	1M KOH	2.25*	[S17]
V_O-Co_3O_4	100	1M KOH	2.30*	[S18]
FeNi-LDH@Ni/SS	100	1M KOH	2.30*	[S19]
Ni-Fe-P@CNTs-CC	100	1M KOH	2.35*	[S20]
NiFe-NC	100	1M KOH	2.35*	[S21]
Co-BTC	100	1M KOH	2.50*	[S22]
This work	100	1M KOH	2.22	/

* The value was estimated according the LSV curves.

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