Supporting Information

Ni single-atom anchored N-doped carbon deposited on $BaTiO_3$ for efficient piezocatalytic CO_2 reduction

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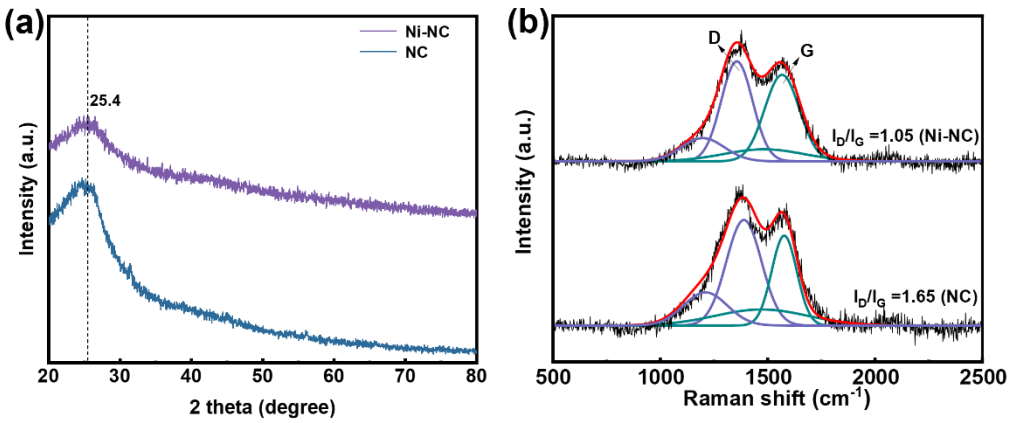

Fig. S1 (a) XRD patterns and (b) Raman spectra of Ni-NC and NC.

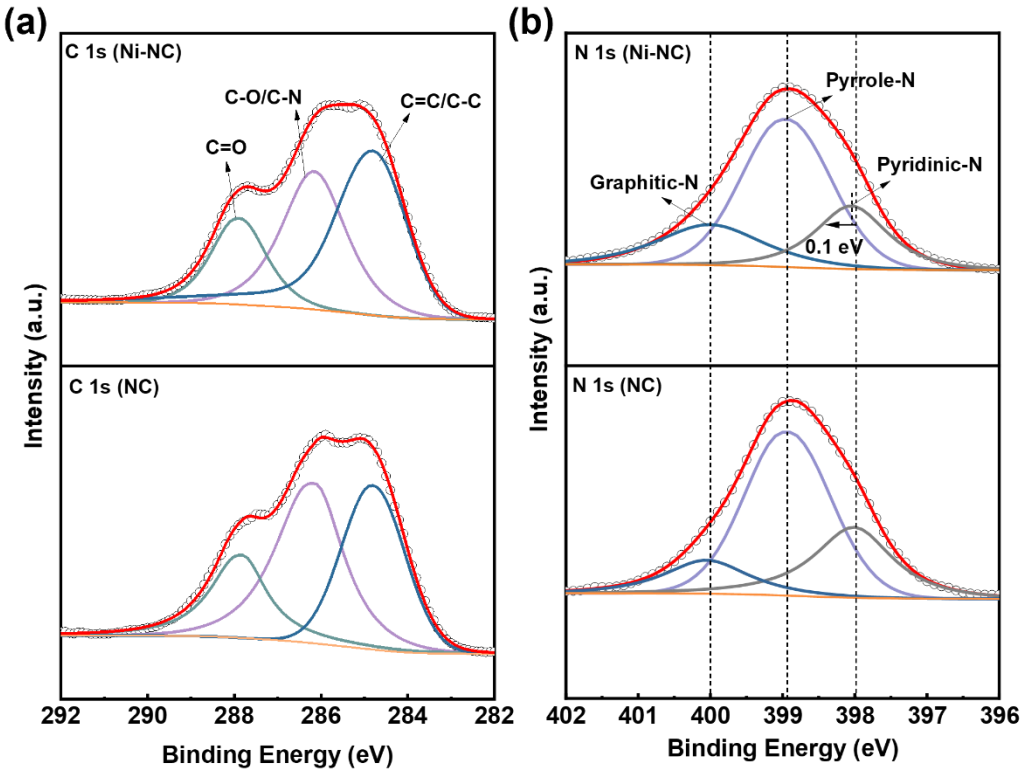

Fig. S2 (a) C 1s and (b) N 1s XPS spectra of Ni-NC and NC.

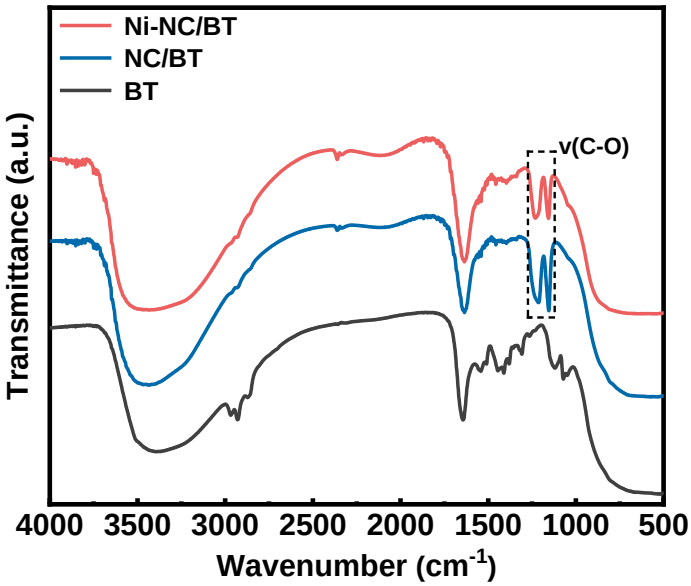

Fig. S3 FT-IR of BT, NC/BT and Ni-NC/BT.

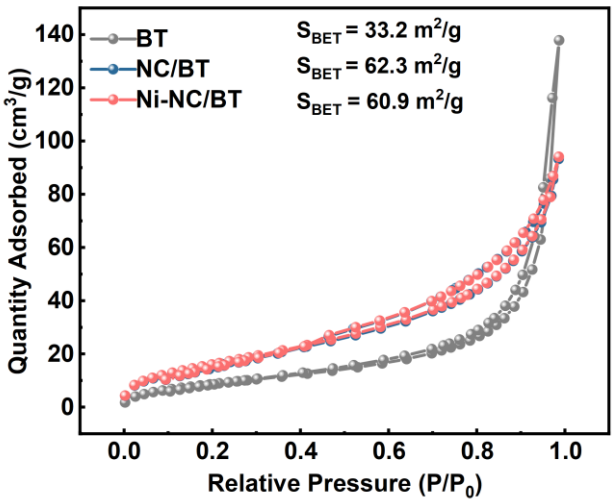

Fig. S4 N_2 adsorption-desorption isotherms and BET surface areas of Ni-NC/BT, NC/BT, and BT.

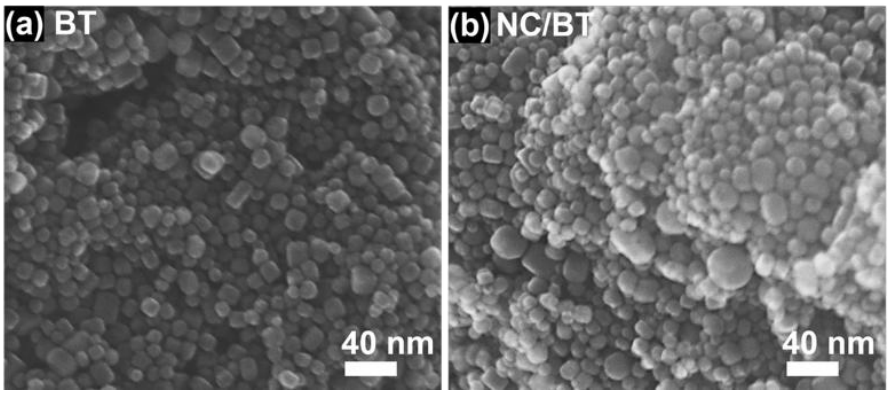

Fig. S5 FE-SEM images of (a) BT and (b) NC/BT.

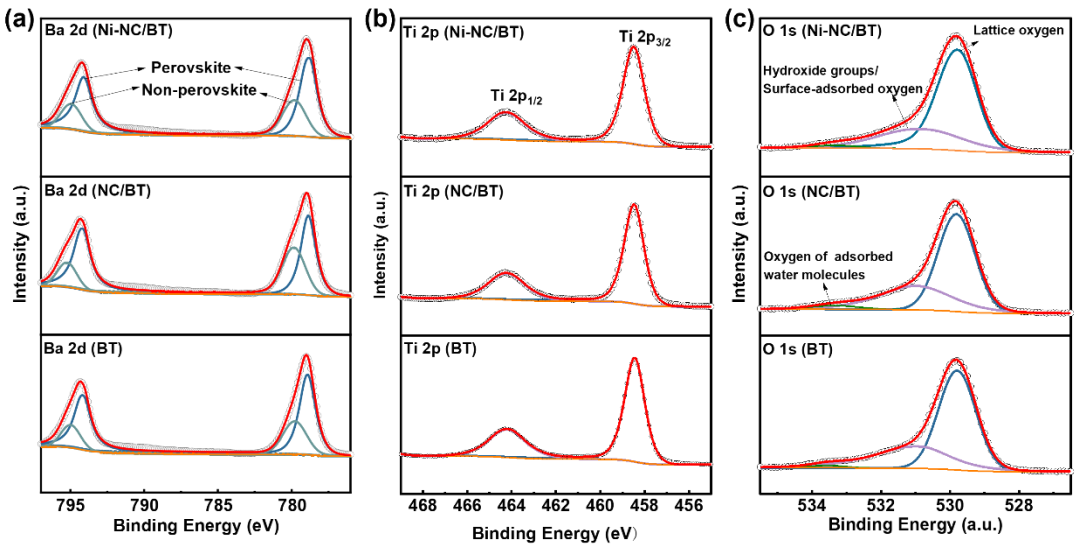

Fig. S6 (a) Ba 2d, (b) Ti 2p and (c) O 1s XPS spectra of Ni-NC/BT, NC/BT, and BT.

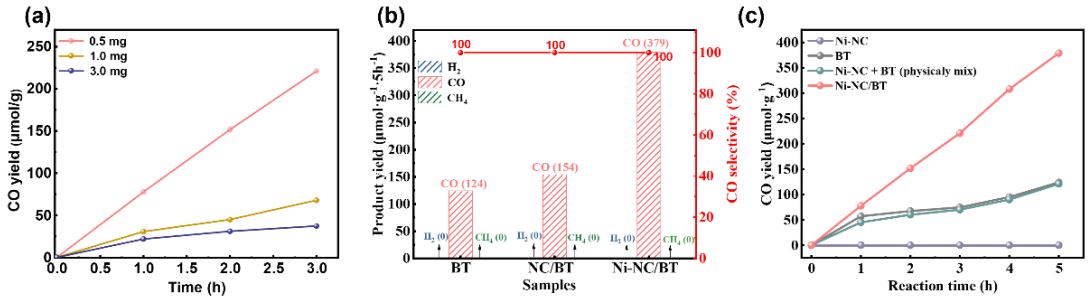

Fig. S7 (a) Time dependence in piezocatalytic CO production using Ni-NC/BT under sonication with different catalyst amounts. (b) Performance testing of piezocatalytic CO production for BT and Ni-NC, and Ni-NC in 5 h of sonication. (c) Time dependence in piezocatalytic CO production over BT, NC/BT, Ni-NC/BT, and physical mixture of and Ni-NC and BT.

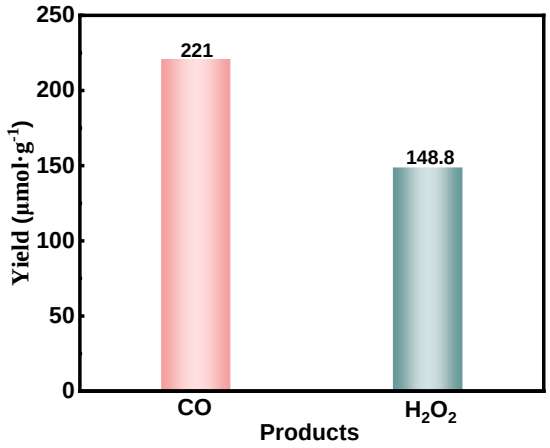

Fig. S8 Performance testing of piezocatalytic CO and H_2O_2 production for Ni-NC/BT in 3h of sonication.

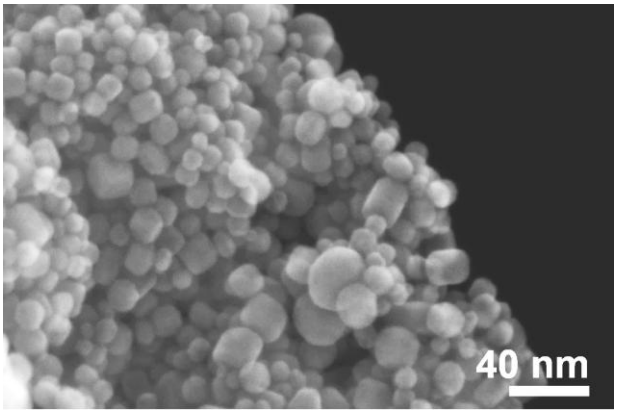

Fig. S9 FE-SEM image of Ni-NC/BT after three cycles of piezocatalytic CO_2 reduction.

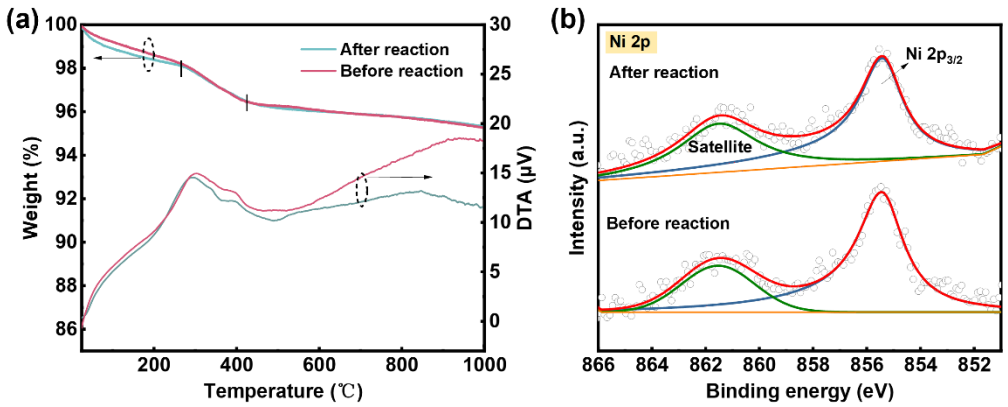

Fig. S10 (a) TG-DTA curves of Ni-NC/BT before and after reaction, and (b) Ni $2p_{3/2}$ XPS spectra of large amount of Ni-NC deposited on BT before and after reaction.

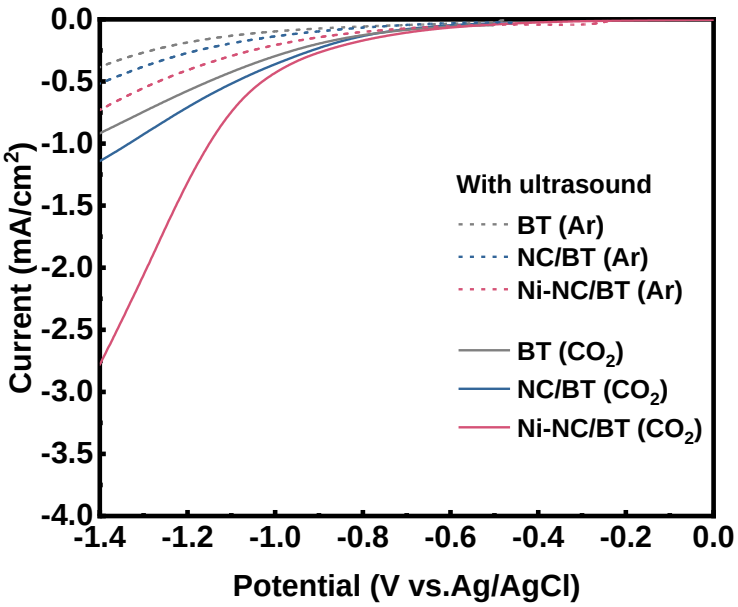

Fig. S11 CO_2 and Ar atmosphere with sonication for BT, NC/BT, and Ni-NC/BT.

Table S1 FT-EXAFS fitting parameters at the Ni K-edge for various samples.

Sample	Path	CN[a]	S_0^2	R(Å)[b]	σ^2(Å^2)[c]	ΔE_0(eV)[d]	R factor
Ni foil	Ni-Ni	12*	0.786	2.4827	0.00597	6.456	0.0015
Ni Pc	Ni-N	4*	0.853*	1.920	0.002	2.775	0.0036
Ni-NC	Ni-N	4.3	0.853*	2.05	0.001	-8.066	0.0155

[a]*CN*, coordination number.

[b]*R*, the distance to the neighboring atom.

[c]σ^2, the Mean Square Relative Displacement (MSRD).

[d]ΔE_0, inner potential correction.

R factor indicates the goodness of the fit.

S_0^2 was fixed to 0.853 according to the experimental EXAFS fit of Ni Pc reference by fixing coordination numbers as the known crystallographic value.

Fitting range: $3.0 \leq k$ (Å) ≤ 12 and $1.0 \leq R$ (Å) ≤ 3.0 (Ni-NC). A reasonable range of EXAFS fitting parameters: $0.800 < S_0^2 < 1.000$; $CN > 0$; $\sigma^2 > 0$ Å^2; $|\Delta E_0| < 10$ eV; *R* factor < 0.02.

Table S2 Comparison of the CO production rates of different catalysts in piezocatalysis.

Piezocatalysts	Energy source	Reaction condition	Main products ($\mu mol \cdot h^{-1} \cdot g^{-1}$)	Ref.
Ni-NC/BT	55W, 48 kHz	0.5 mg sample +15 mL DI	75.8	This work
$BaTiO_3$/GO	120 W, 80 kHz	1 mg sample+5 mL of 0.35 M $Na_2S \cdot 9H_2O$ and 0.25 M Na_2SO_3	134.4	1
Au/ZnO	120 W, 80 kHz	5 mg sample+10 mL of 0.35 M $Na_2S \cdot 9H_2O$ and 0.25 M Na_2SO_3	88.7	2
Co-N-C@$BaTiO_3$	300 W, 50 kHz	40 mg sample+500 mL of 0.1 M $KHCO_3$ (pH=8.57) solution	261.8	3
Li-doped potassium sodium niobate (KNLN)	60 W, 50 kHz	10 mg KNLN+10mLof 0.1M Na_2SO_3	438	4
$BaTiO_3$	0.7 W/cm^2, 40 kHz	5mg sample + 5 mL DI 5mg sample + 5 mL DI +0.35 M $Na_2S \cdot 9H_2O$ and 0.25 M Na_2SO_3	3.4 63.3	5
MoS_2	100 W, 40 kHz	5 mg sample + 5 mL DI+ (sacrificial agent) 0.35 M $Na_2S \cdot 9H_2O$ and 0.25 M Na_2SO_3	543.1	6
Nb doped PZT	40 kHz	10 mL of 0.1 M Na2SO3	789	7
BiFeO3−x	100 Hz	12 mg sample + 2 mL of DI+22 mL acetonitrile + 6 mL triethanolamine	8.87	8
$Bi_7Ti_4NbO_{21}$ nanosheets	240 W,40 kHz	10mg sample + 100 mL of DI	19.10	9

Table S3 The performance comparison of piezocatalytic H_2 production via water splitting over different materials.

Piezocatalysts	Energy source	Reaction condition	Main products ($\mu mol \cdot h^{-1} \cdot g^{-1}$)	Ref.
Ni-NC/BT			4140	This work
NC/BT	55W, 48 kHz	0.5 mg sample +15 mL DI	2628	This work
BT			1820	This work
10nm $BaTiO_3$	40 kHz	5 mg sample + 10 mL DI	655	10
V-$NaNbO_3$	192 W, 68 kHz	10 mg sample + 45 mL DI	346.2	11
ZnS NSs	100 W, 27 kHz	5 mg sample+ 10 mL DI	1080	12
C doped $KNbO_3$	-	50 mg sample + 25 mL DI	524.51	13
$Bi_4O_5Br_2$	240, 4 kHz	10 mg sample + 100 mL DI	1149	14
Co_4N-WN_x	~75 kHz	4 mg sample + 10 mL DI	262.7	15
$Bi_2Fe_4O_9$	200 W, 40 kHz	2 mg sample + 10 mL DI	1058	16
Bi_4TaO_8Cl	110 W, 37 kHz	10 mg sample + 30 mL DI	1500	17
H/C-CdS	240 W, 40 kHz	2 mg sample + 15 mL DI	3190	18
$BiFeO_3$@COF	100 W, 40 kHz	5 mg sample + 10 mL DI	1416.4	19
$RbBiNb_2O_7$/ poly(tetrafluoroethylen)	240 W, 68 kHz	20 mg sample + 30 mL DI	260.79	20
N doped MoC	100 W, 40 kHz	10 mg sample + 20 mL DI	1690	21
C_3N_4@Ag	180 W, 40 kHz	2 mg sample + 100 mL DI	7900	22
$Bi_4Ti_3O_{12}$@Au	100 W, 40 kHz	20 mg sample + 10 mL DI	194.67	23
g-C_3N_4	240 W, 40 kHz	2 mg sample + 100 mL DI	8970	24
La_2NiO_4	70 W, 40 kHz	10 mg sample + 80 mL DI	1097	25
$BaTiO_{3-x}$	100 W, 40 kHz	100 mg sample +100 mL DI	132.4	26
Bi_2MoO_6-$BaTiO_3$	300 W	50 mg sample +200 mL DI	152.57	27

Table S4 Elemental analysis of Ni-NC/BT before and after reaction.

Sample	Ni/(Ni+Ba+Ti)* (mol%)
Ni-NC/BT (before reaction)	0.56
Ni-NC/BT (before reaction)	0.49

*Determined from XRF analysis

Table S5 Summarizes the values of E_g, VB_{max}, E_{VB}, and E_{CB} of BT, NC/BT, and Ni-NC/BT.

Samples	E_g (eV)	VB_{max} (E_f, V vs. NHE)	E_{VB} (V vs. NHE)	E_{CB} (V vs. NHE)
BT	3.54	2.66	2.72	-0.88
NC/BT	3.47	2.64	2.70	-0.83
Ni-NC/BT	3.45	2.59	2.65	-0.86

*$E_{NHE} = \Phi + E_f - 4.44$ (where E_{NHE} is the standard electrode potential and Φ is the work function of XPS, which is 4.5 eV in this work)[28]

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