Electronic Supplementary Material (ESI)

Powerful CO2 electroreduction performance with N-carbon doped by Ni single atoms

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Supporting Figures

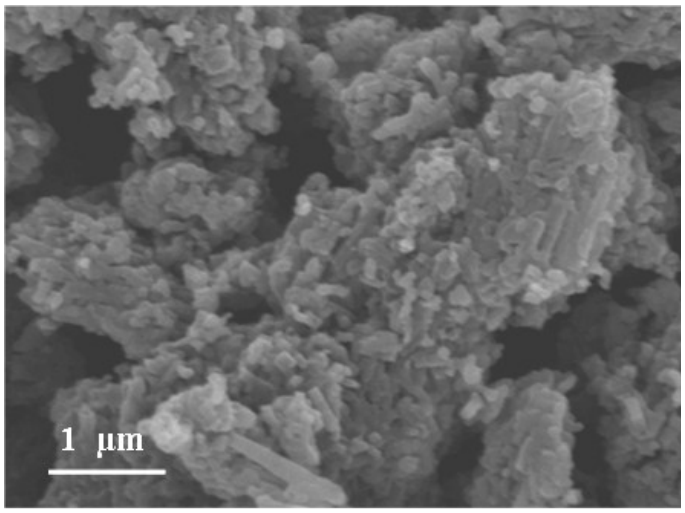

Fig. S1 The SEM image of the obtained N-C sample.

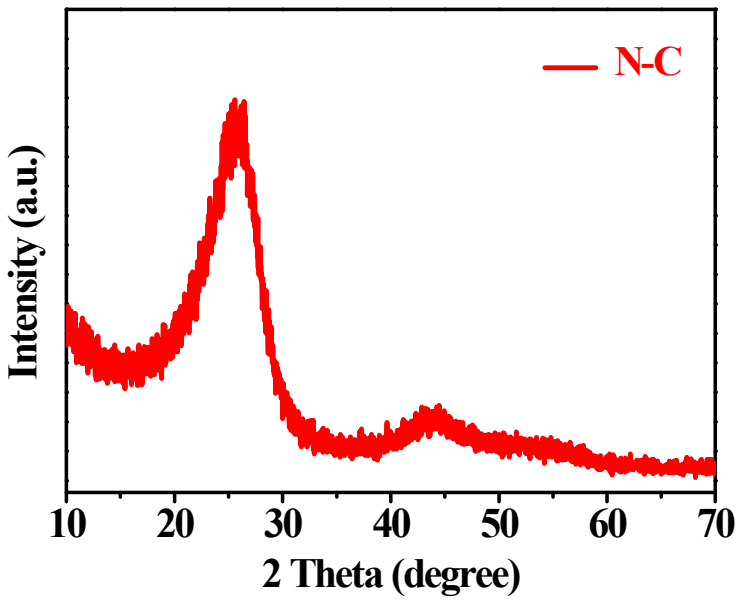

Fig. S2 The XRD pattern of the obtained N-C sample.

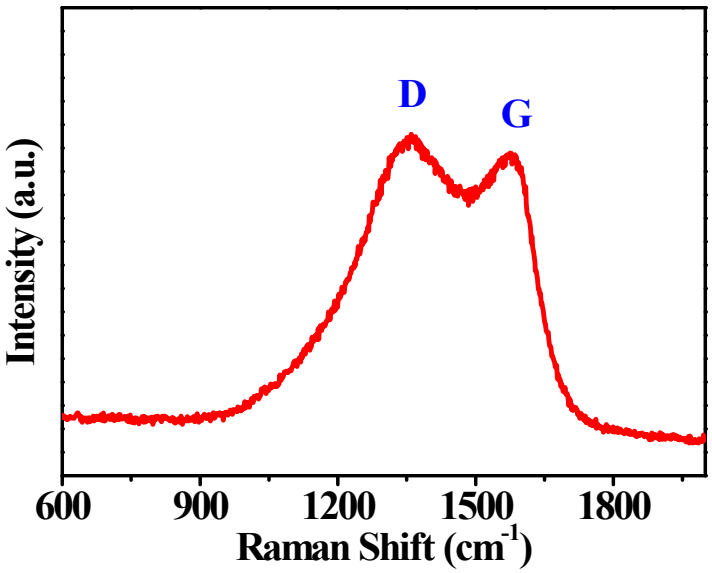

Fig. S3 The Raman spectrum of the obtained Ni-N-C sample.

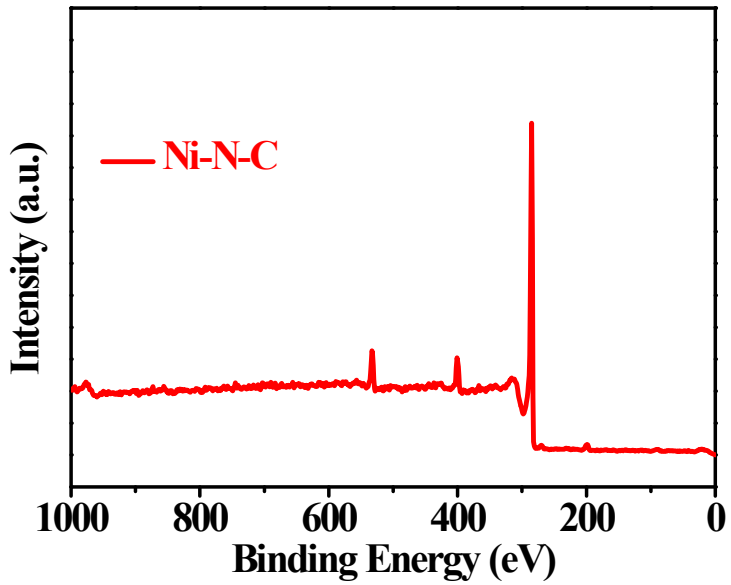

Fig. S4 The survey XPS spectrum of the Ni-N-C sample.

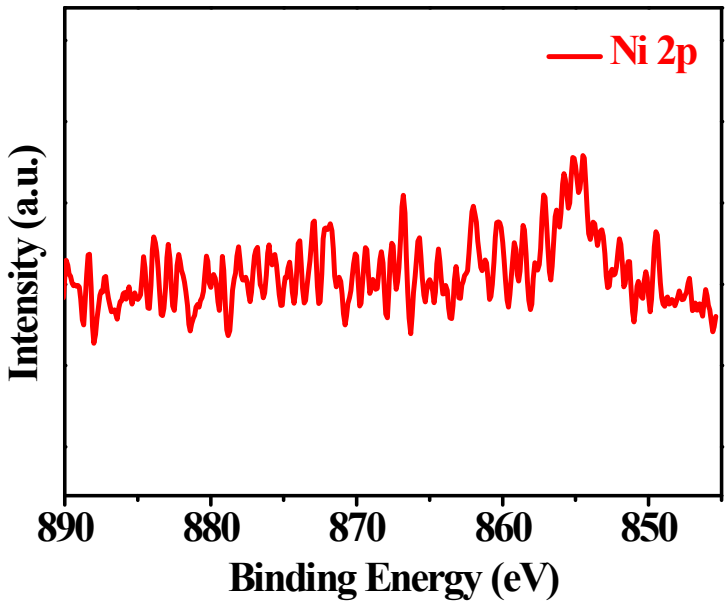

Fig. S5 The high-resolution Ni 2p XPS spectrum of the Ni-N-C catalyst.

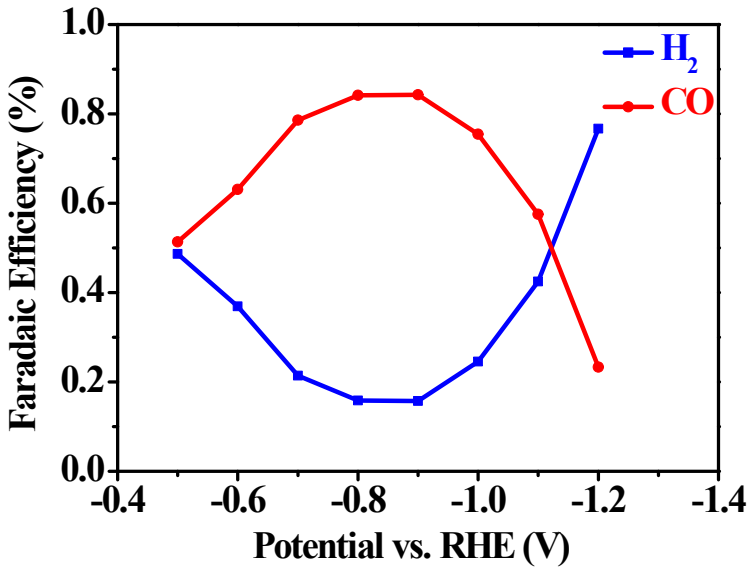

Fig. S6 The CO_2RR performance of the controlled sample prepared using pure Zn-bidppz without the adding of Ni as precursor.

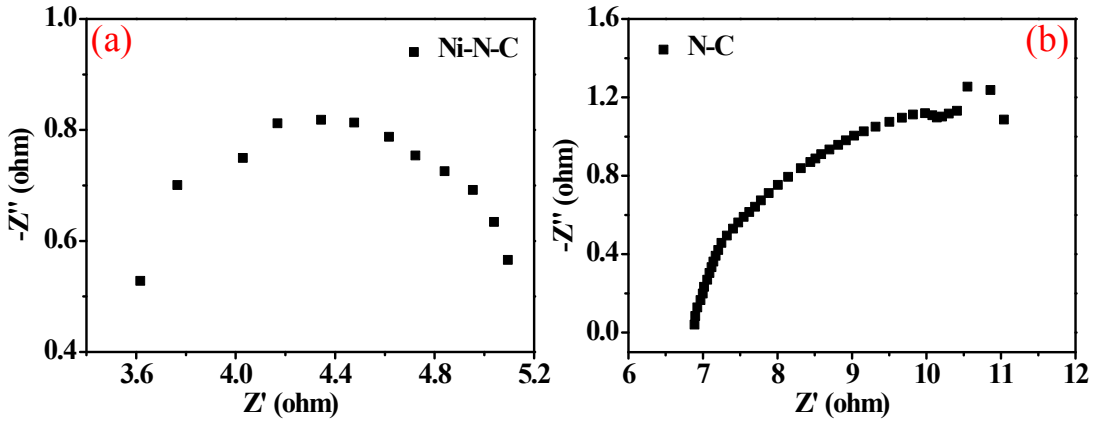

Fig. S7 The Nyquist plots of Ni-N-C (a) and N-C (b) catalysts.

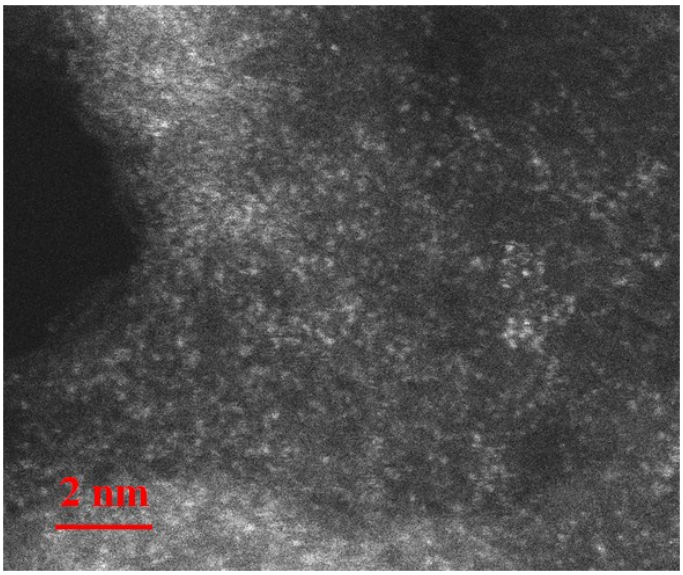

Fig. S8 The HAADF-STEM image of Ni-N-C catalyst after electrocatalysis.

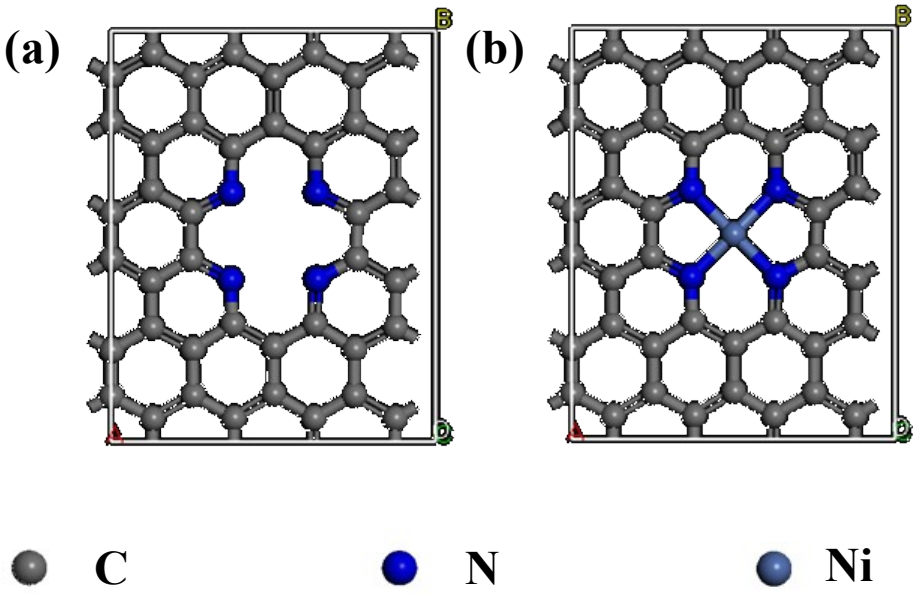

Fig. S9 The optimized structures of N-C (a) and Ni-N-C (b).

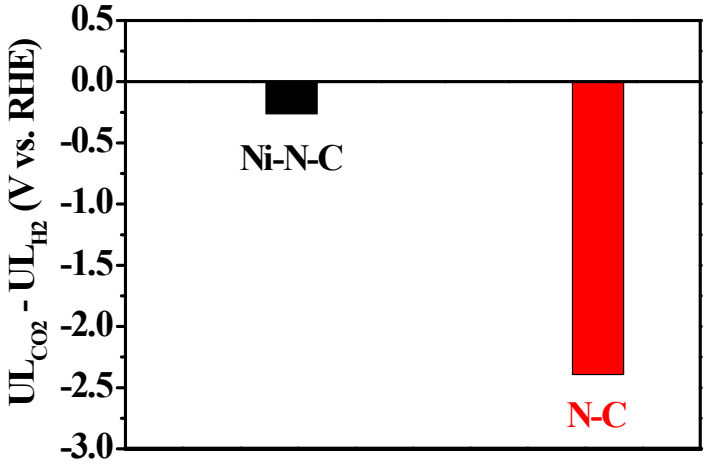

Fig. S10 The difference in limiting potentials for CO_2 reduction and H_2 evolution of N-C and Ni-N-C.

Table S1 Structural parameters of Ni-N-C extracted from the EXAFS fitting (S_0^2=0.85).

Sample	Scattering pair	CN	R(Å)	σ ^{2}(10^{-3}Å^2)	ΔE_0(eV)	R factor
Ni-N/C	Ni -N	3.9±1.1	1.90±0.02	6.6±1.7	5.6±1.4	0.0073

S_0^2 is the amplitude reduction factor; CN is the coordination number; R is interatomic distance (the bond length between central atoms and surrounding coordination atoms); σ^2 is Debye-Waller factor (a measure of thermal and static disorder in absorber-scatterer distances); ΔE_0 is edge-energy shift (the difference between the zero kinetic energy value of the sample and that of the theoretical model). R factor is used to value the goodness of the fitting.

Table S2 The Zero point energy (ZPE) corrections and entropic contributions to the free energies.

		ZPE/eV	TS/eV
CO_2		0.2673	0.6606
COOH *	C-N	0.5725	$8.839X10^{-3}$
	Ni-C-N	0.5281	0.0128
CO *	C-N	0.1291	$1.23X10^{-5}$
	Ni-C-N	0.1227	$1.93X10^{-5}$
H_2O (l)		0.5681	0.67
CO		0.1317	0.6108
H*	C-N	0.307	$2.121X10^{-3}$
	Ni-C-N	0.3112	$2.557x10^{-3}$
H_2		0.2689	0.4038