

Supporting Information for:

Structural Evolution of CrN Nanocube Electrocatalysts during Nitrogen Reduction Reaction

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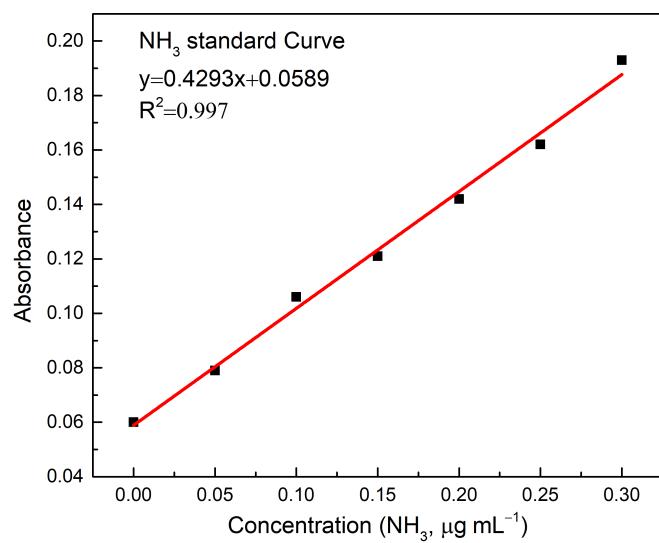


Fig. S1 Calibration curve used for estimation of NH₃ concentration.

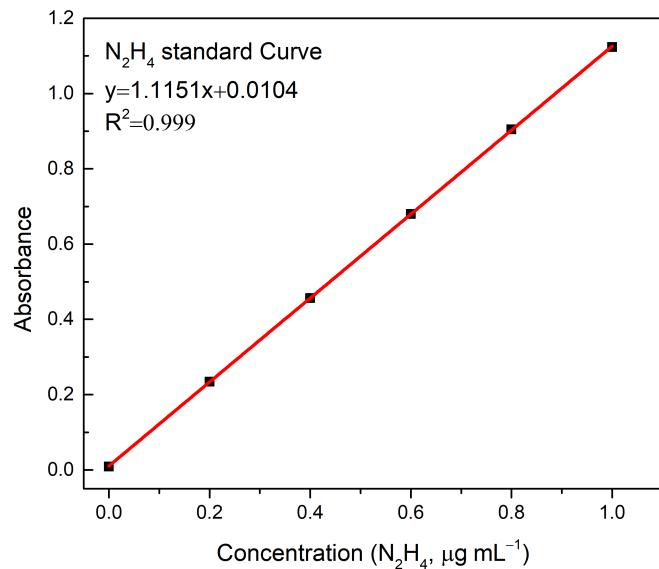


Fig. S2 Calibration curve used for estimation of N₂H₄ concentration.

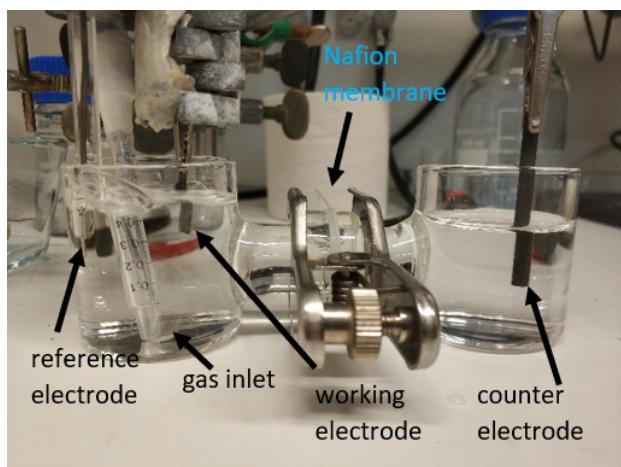


Fig. S3 Photographic of the electrocatalytic device.

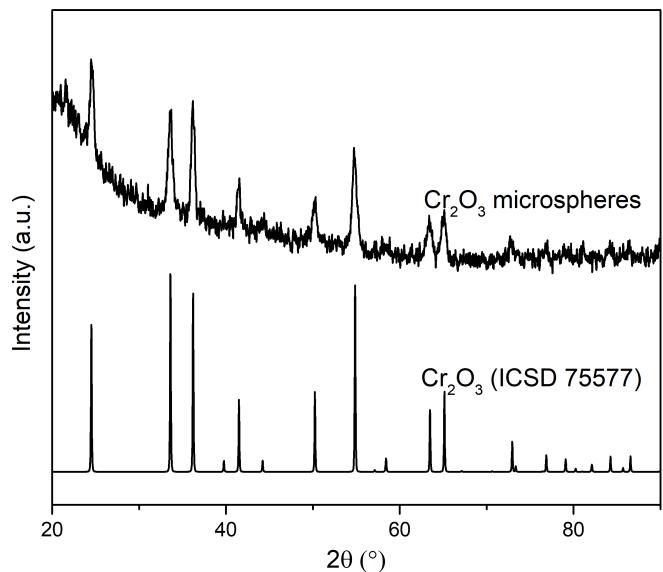


Fig. S4 Experimental and simulated powder XRD patterns of Cr₂O₃ microspheres (ICSD 75577).

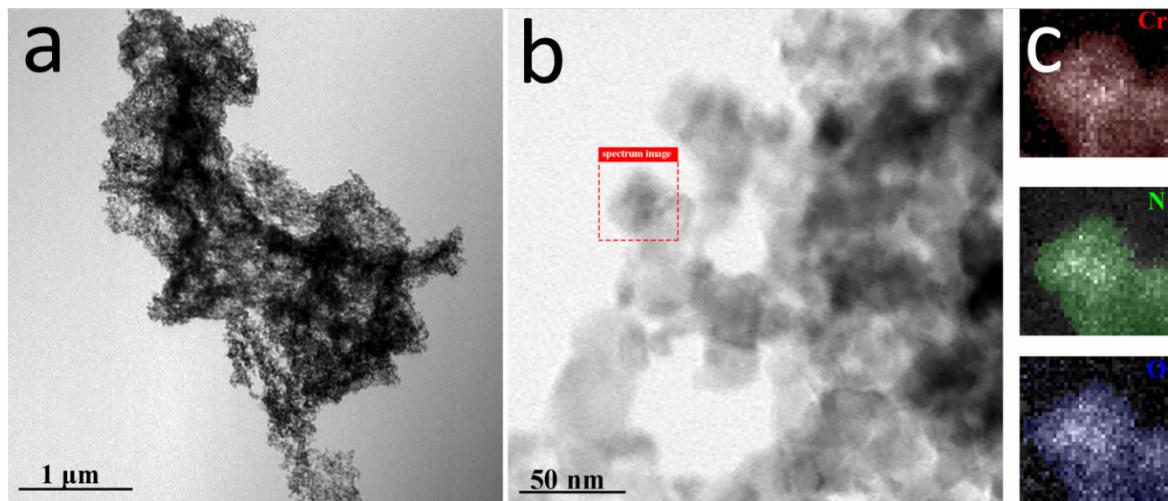


Fig. S5 STEM images (a, b) of as-prepared CrN NCs and STEM EDX mapping (c) for as-prepared CrN NCs.

II. Supplemental Table

Table S1 Summary of the representative reports on electrocatalytic NRR at ambient conditions.

Catalyst	Electrolyte	NH ₃ yield	FE(%)	Ref.
CrN nanocubes	0.1 M HCl	31.11 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	16.64	This work
VN	0.1 M HCl	$8.40 \times 10^{-11} \text{ mol s}^{-1}\text{cm}^{-2}$	2.25	¹
mesoporous boron nitride	0.1 M Na ₂ SO ₄	18.2 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	5.5	²
MoN	0.1 M HCl	$3.05 \times 10^{-10} \text{ mol s}^{-1}\text{cm}^{-2}$	1.15	³
defect-rich MoS ₂	0.1 M Na ₂ SO ₄	29.28 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	8.34	⁴
hollow Cr ₂ O ₃ microspheres	0.1 M Na ₂ SO ₄	25.3 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	6.78	⁵
Cr ₂ N	-	$1.40 \times 10^{-11} \text{ mol s}^{-1}\text{cm}^{-2}$	0.58	⁶
Nb ₃ O ₇ (OH)	0.1 M Na ₂ SO ₄	622 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	39.9	⁷
TiO _x N _y	0.1 M Na ₂ SO ₄	4.1 mg $\text{h}^{-1} \text{g}_{\text{cat.}}^{-1}$	9.1	⁸
np-PdH _{0.43}	0.1 M PBS	20.4 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	43.6	⁹
3D Rh	0.1 M KOH	35.58 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	0.52	¹⁰
Mo-doped W ₁₈ O ₄₉	0.1 M Na ₂ SO ₄	5.3 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	12.1	¹¹
multi-yolk-shell bismuth@porous carbon	0.1 M HCl	28.63 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	10.58	¹²
α -Fe ₂ O ₃ @mTiO ₂ -400	0.1 M Na ₂ SO ₄	27.2 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	13.3	¹³
Ti ₃ C ₂ T _x QDs	0.1 M HCl	62.94 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	13.30	¹⁴
amorphous FeB ₂ porous nanosheets	0.5 M LiCO ₄	39.8 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	16.7	¹⁵
Cu-TiO ₂	0.5 M LiCO ₄	21.31 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	21.99	¹⁶
Co-SAs/NC	0.005 M H ₂ SO ₄	16.9 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	18.8	¹⁷
CoS ₂ @NC	0.1 M HCl	17.45 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	4.6	¹⁸
MV-MoN@NC	0.1 M HCl	76.9 $\mu\text{g h}^{-1} \text{mg}_{\text{cat.}}^{-1}$	6.9	¹⁹

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