Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

Transition-metal nitride nanoparticles embedded in N-doped reduced graphene oxide: Superior synergistic electrocatalytic materials for counter electrodes of dye-sensitized solar cells

Xiaoying Zhang, [a, b, ‡] **Xiao Chen,** [a, ‡] **Kejun Zhang,** [a, b] **Shuping Pang,** [a] **Xinhong Zhou,**[c] **Hongxia Xu,** [a] **Shanmu Dong,** [a] **Pengxian Han,** [a] **Zhongyi Zhang,** [a, b] **Chuanjian Zhang,** [a, b] **Guanglei Cui** [a,*]

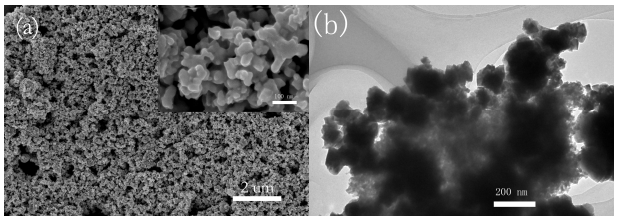


Fig. 1S Typical low magnification SEM (a) and TEM (b) images of bare MoN surface; The inset corresponds to the corresponding high magnification SEM.

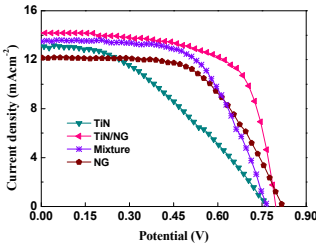


Fig. 2S Photocurrent-voltage (*J-V*) curves of the DSCs with different couter electrodes of TiN nanoparticles, pristine NG, TiN/NG hybrids and Mixture under 1 sun (AM 1.5) illumination.

Fig. 2S and Table S1 reveal that all the photovoltaic parameters of DSC using TiN/NG are higher than those of the DSCs using the Mixture (physical mixture of TiN and NG), highlighting the predominant synergic effect of NG and nitrides nanoparticles. Their elecrocatalytic activity was evaluated by CV (**Fig.** 3 S).

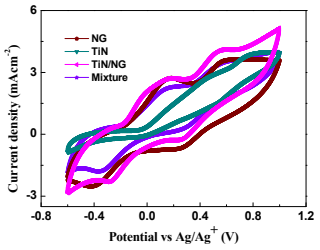
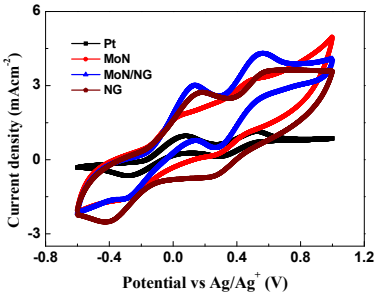
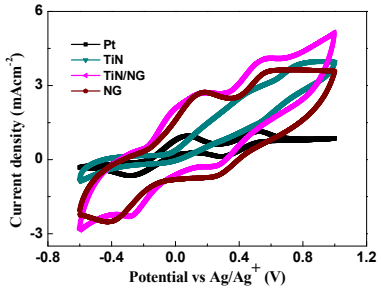


Fig. 3S Cyclic voltammograms of various counter electrodes at a scan rate of 20 mVs^{-1} in 10 mM LiI, 1 mM I_2 acetontrile solution containing 0.1 M LiClO4 as the supporting electrolyte.





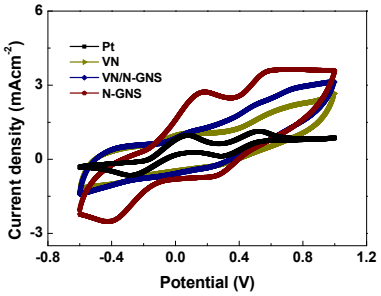


Fig. 4S Cyclic voltammograms of various counter electrodes at a scan rate of 20 mVs^{-1} in 10 mM LiI, 1 mM I_2 acetontrile solution containing 0.1 M LiClO4 as the supporting electrolyte.

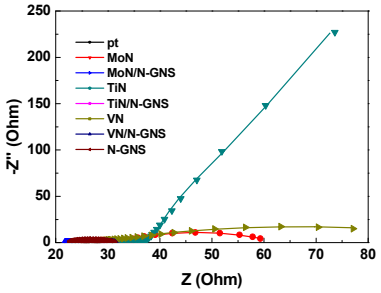


Fig. 5S Impedance spectra of the symmetric cells with two identical counter electrodes of nitrides (MoN, TiN, VN) nanoparticles, pristine NG, (MoN, TiN, VN)/NG hybrids and Pt in the measured frequency range from 100 kHz to 100 mHz. The symbols and lines correspond to the experimental and simulated data, respectively.

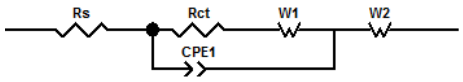


Fig. 6S The conventional equivalent circuit of the symmetric cell. When the simulation is carried out for Pt CE,W1 is excludeed in the equivalent circuit above. R_S: series resistance; R_{ct}: charge transfer resistance; W1: Nernst diffusion impedance within electrode pores; CPE1: constant phase element of one electrode, W2: Nernst diffusion impedance between the electrodes.

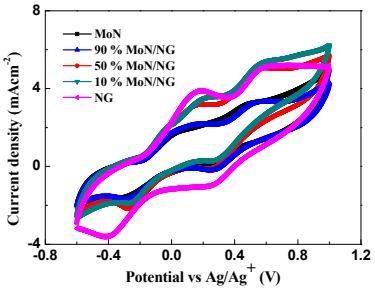


Fig. 7S Cyclic voltammograms of various MoN/NG with different feed ratio at a scan rate of 20 mVs^{-1} in 10 mM LiI, 1 mM I_2 acetontrile solution containing 0.1 M $LiClO_4$ as the supporting electrolyte.

Table 1S photovoltaic parameters of DSCs based on various counter electrodes.

Samples	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	η (%)
TiN	0.768	13.04	30.72	3.078
TiN/NG	0.796	14.16	66.52	7.498
Mixture	0.769	13.60	60.28	6.306
NG	0.821	12.14	58.21	5.800

Table 2S Fitted electrochemical parameters from Electrochemical Impedance Spectra (EIS)

parameter	R ($\Omega\ cm^{-2}$)	CPE		R ($\Omega\ cm^{-2}$)	W1 ($\Omega\ cm^{-2}$)		W2 ($\Omega\ cm^{-2}$)	
		Y0	n		Y0	B	Y0	B
Pt	23.70	5.51E-05	0.87	6.557	-	-	0.5005	1.056
MoN	24.88	1.00E-03	0.84	6.563	2.80E-01	1.6	0.0279	0.67
MoN/NG	21.67	2.13E-04	0.77	1.393	8.97E-01	0.65	0.2718	0.17
TiN	28.01	2.82E-04	0.63	9.647	7.71E-02	0.01	0.02509	0.43
TiN/NG	25.16	3.23E-05	0.86	2.211	3.43E-02	0.05	1.263	0.78
VN	26.26	1.09E-02	0.55	7.44	3.06E+13	62.75	0.01698	0.05
VN/NG	25.83	7.93E-06	0.97	1.623	2.33E-02	0.07	1.403	97.91
NG	22.57	2.47E-05	0.80	8.177	2.24E+18	0.01	0.6754	0.14

Table 3S The practical MoN loading amounts in MoN/NG hybrids with different feed ratio.

Samples	MoN (%)
NG	0
10 % MoN/NG	28.26
50 % MoN/NG	51.36
90 % MoN/NG	84.83
MoN	100