Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information:

Rational design of M–N_4–Gr/V_2C heterostructures as highly active ORR catalysts: A density functional theory study

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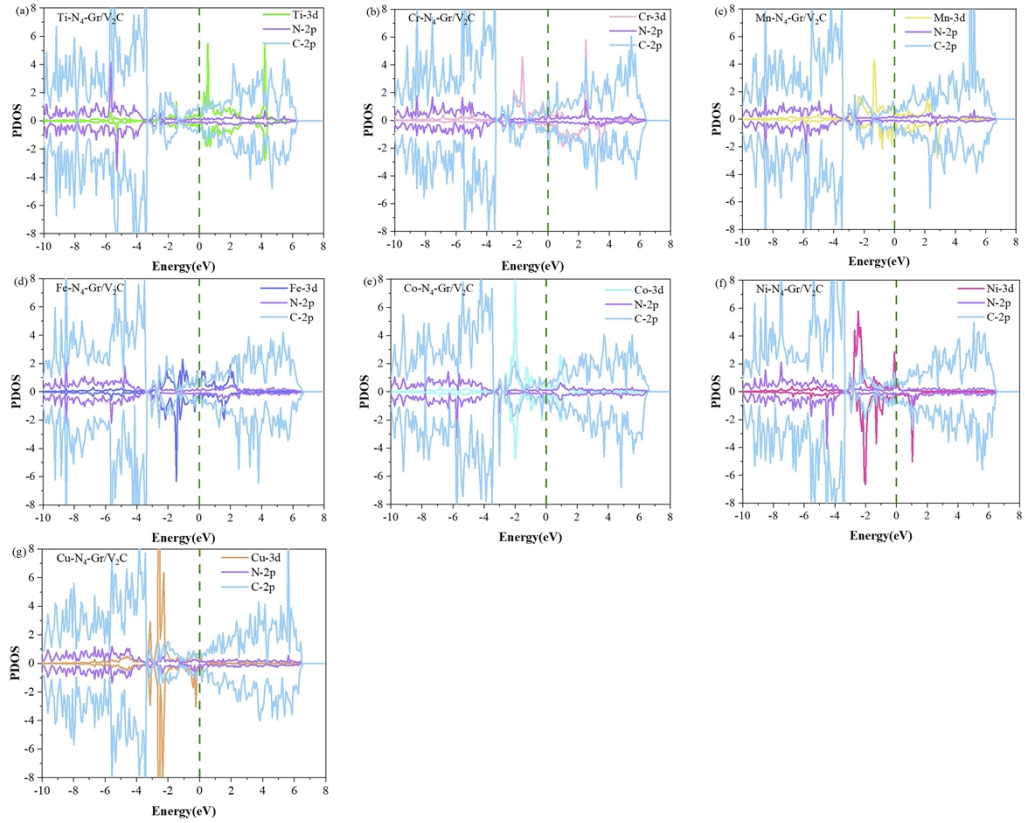

Fig. S1 The dos plots of M-3d, N-2p, C-2p for (a-g) M-N_4-Gr/V_2C（M=Ti, Cr, Mn, Fe, Co, Ni, Cu）. The dotted line at zero represents the Fermi energy level.

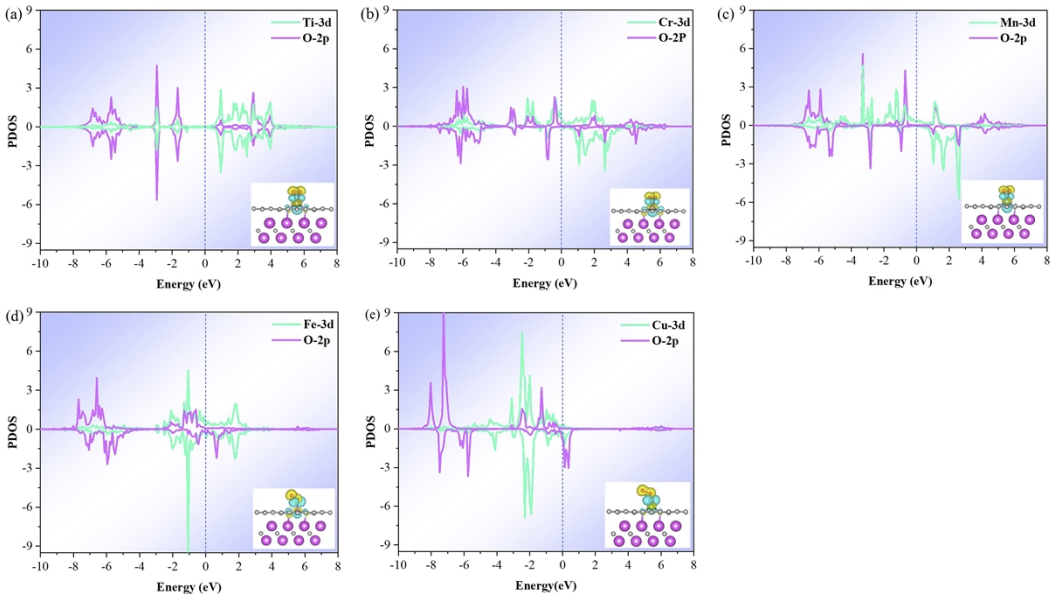

Fig. S2 PDOS of O_2 adsorbed on (a-e) M-N_4-Gr/V_2C (Ti, Cr, Mn, Fe, Cu) catalysts with M-3d and O-2p. The inset is a distribution of exchange charges between O_2 and M-N_4-Gr/V_2C with the isovalue of 0.054 e$Å^{-3}$. The blue and yellow bubbles represent positive and negative charges, respectively.

Table S1 With or without V_2C as substrate material M charge transfer amount(Q-$_M$(e)).

Properties	Q-$_M$(e)	Properties	Q-$_M$(e)
Ti-N_4-Gr	1.66	Ti-N_4-Gr/V_2C	1.39
Cr-N_4-Gr	1.32	Cr-N_4-Gr/V_2C	0.99
Mn-N_4-Gr	1.37	Mn-N_4-Gr/V_2C	0.76
Fe-N_4-Gr	1.10	Fe-N_4-Gr/V_2C	0.63
Co-N_4-Gr	0.90	Co-N_4-Gr/V_2C	0.61
Ni-N_4-Gr	0.86	Ni-N_4-Gr/V_2C	0.62
Cu-N_4-Gr	0.94	Cu-N_4-Gr/V_2C	0.70