Supporting information

Tuning sp-hybridized N anchored the single atom on graphdiyne for efficient oxygen reduction reaction: A DFT study

Ning Wang[1], Siyu Gan[1], Yunfeng Mao[2], Junping Xiao[3,*], Chunming Xu[4,5], and Tianhang Zhou[4,5,*]

1 School of Science, Key Laboratory of High-Performance Scientific Computation, Xihua University, Chengdu 610039, China

2 School of Energy and Power Engineering, University of Shanghai for Science and Technology, Shanghai, 200093, China

3 College of Physics and Electronic Information, Baicheng Normal University, Baicheng, Jilin 137000, China

4 College of Carbon Neutrality Future Technology, China University of Petroleum (Beijing), Beijing 102249, China;

5 State Key Laboratory of Heavy Oil Processing, China University of Petroleum (Beijing), Beijing 102249, China

* Correspondence: djtc999@163.com (Junping Xiao); zhouth@cup.edu.cn (Tianhang Zhou)

1. Computational details

The formation energy (ΔE_f) of the N-doping site in GDY is calculated as:

$$\Delta E_f = E(\text{N-doped GDY}) - \frac{m-n}{m} E(\text{GDY}) - \frac{n}{2} E(N_2)$$

where E(N-doped GDY) and E(GDY) are the total energies of the N-doped and original GDY, respectively. $E(N_2)$ is the total energy of an isolated N_2 molecule. m and n are the number of carbon atoms in the original GDY and the number of doped N atoms, respectively.

2. Results

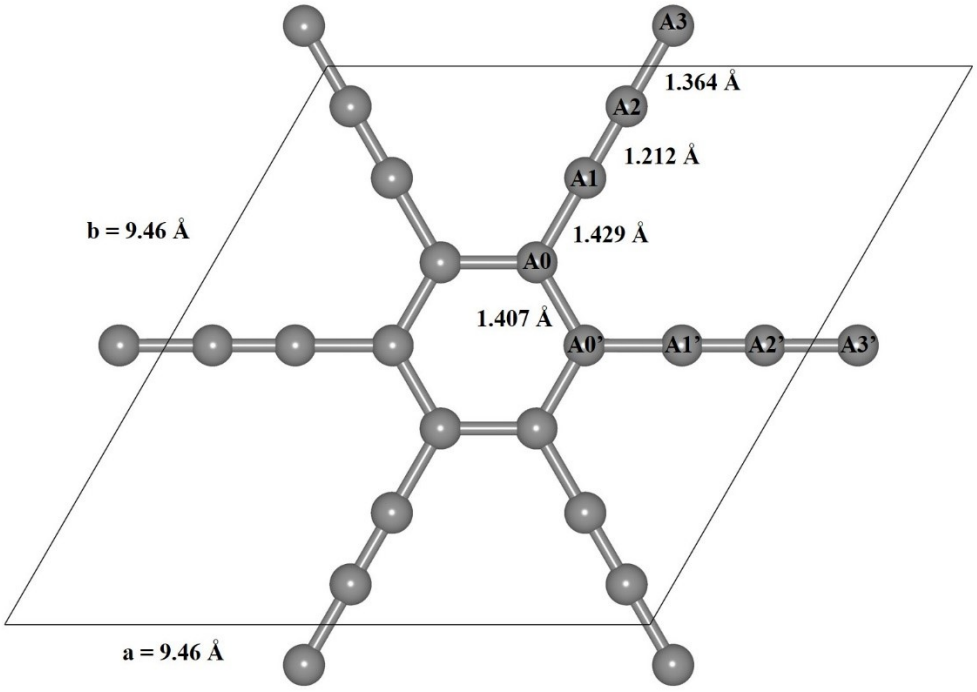
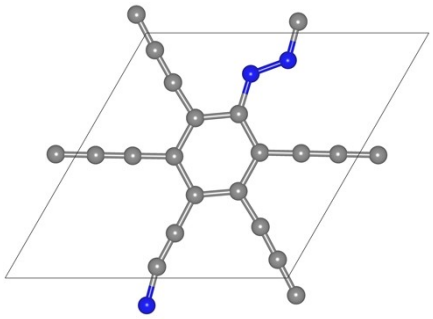
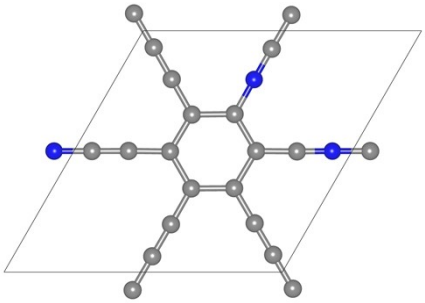
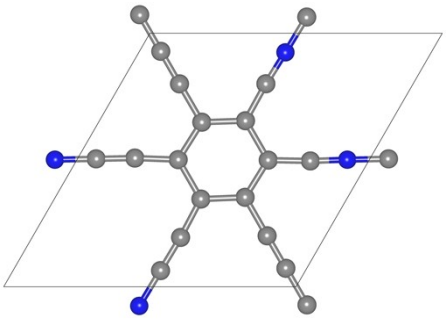
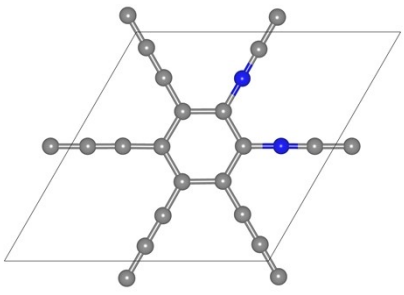


Fig. S1. The structure of pristine GDY. Note that the position of N-doping sites is marked as A1, A1', A2, A2'.

Table S1. Formation energies (ΔE_f) of N-doping sites in GDY.

N-doping sites	Structure	ΔE_f (eV)
A1-A2		1.16
A1-A2’		0.86
A2- A2’		1.00
A1-A1’		0.69

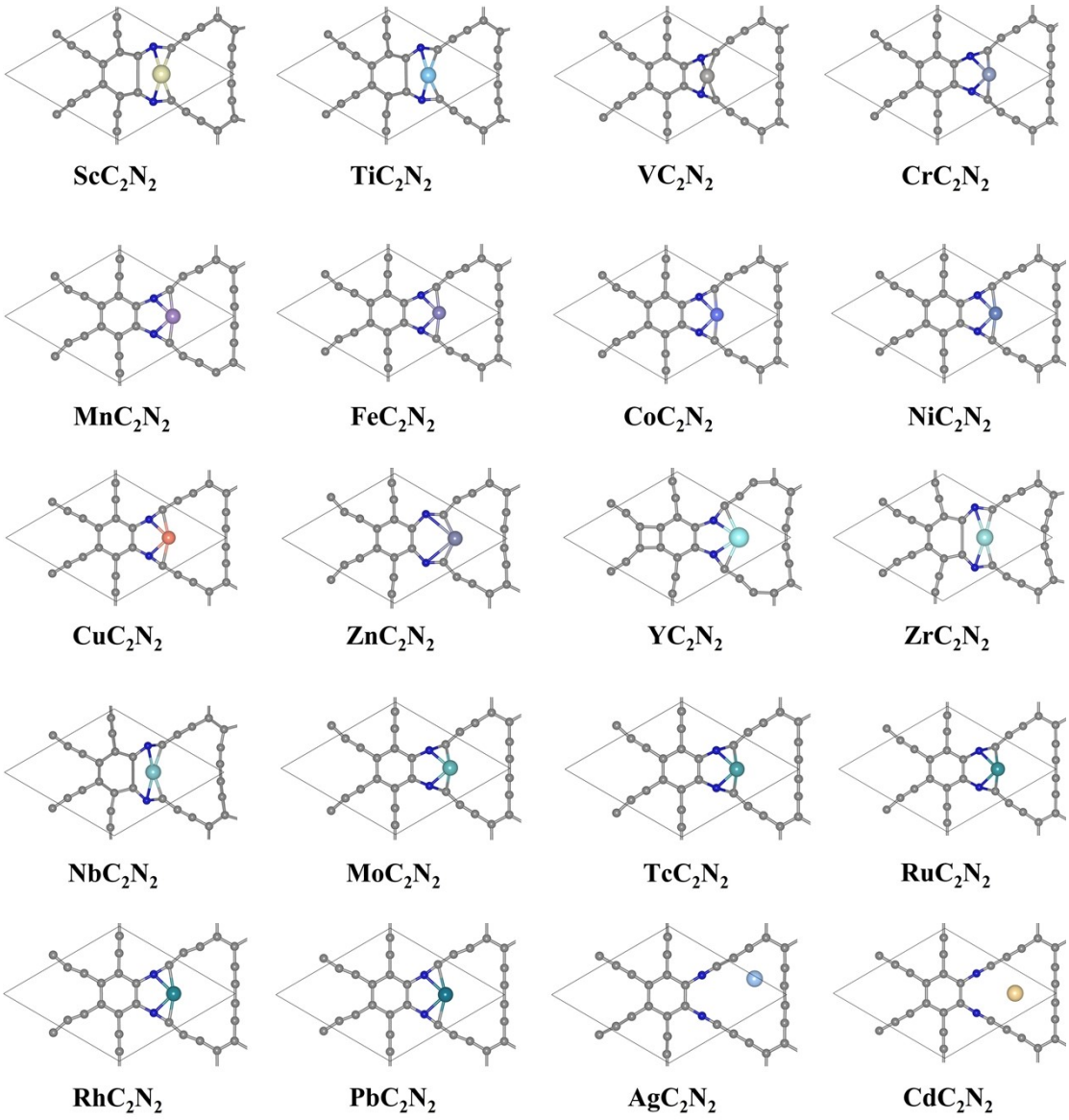


Fig. S2. Optimized structures of TMC_2N_2.

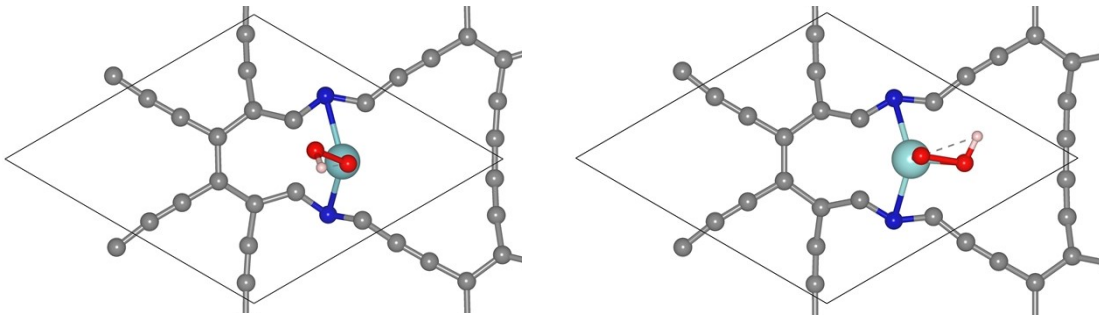


Fig. S3. Configurations of *OOH adsorbed on NbC_2N_2 and ZrC_2N_2.

Table S2. Corresponding free energies of adsorption of *OOH, *O, and *OH on TMC_2N_2 and TMC_2N_2-OH. The values in the brackets are obtained in the H_2O solvent environment.

	before OH ligand modification			after OH ligand modification		
	ΔG_{*OOH}	ΔG_{*O}	ΔG_{*OH}	ΔG_{*OOH}	ΔG_{*O}	ΔG_{*OH}
Sc	2.28(1.93)	-0.23(-0.51)	-0.98(-1.53)	3.48(3.13)	-0.73(-1.05)	0.19(-0.44)
Ti	1.44(1.11)	-0.82(-1.12)	-1.82(-2.44)	3.47(3.13)	0.59(0.32)	0.03(-0.53)
V	1.70(1.35)	-1.34(-1.63)	-1.77(-2.41)	5.32(4.96)	3.84(3.53)	0.55(-0.09)
Cr	2.12(1.84)	-0.71(-1.01)	-1.28(-1.85)	4.66(4.31)	0.41(0.13)	0.37(-0.25)
Mn	2.54(2.24)	-0.39(-0.72)	-0.76(-1.51)	3.42(3.02)	1.32(0.98)	0.84(0.30)
Fe	2.63(2.29)	0.22(-0.05)	-0.88(-1.59)	3.87(3.50)	1.45(1.12)	0.69(0.04)
Co	3.23(2.94)	0.65(0.32)	-0.11(-0.68)	3.28(2.95)	0.87(0.55)	-0.06(-0.64)
Ni	2.72(2.46)	0.35(0.04)	-0.34(-0.96)	3.07(2.73)	0.61(0.32)	0.54(-0.04)
Cu	2.67(2.39)	0.35(0.02)	-0.76(-1.35)	2.71(2.38)	0.66(0.39)	0.67(0.03)
Y	1.73(1.39)	-0.80(-1.08)	-1.96(-2.53)	3.37(3.03)	2.90(2.58)	0.02(-0.60)
Mo	1.41(1.07)	-0.96(-1.21)	-1.61(-2.25)	3.19(2.85)	0.28(-0.04)	-0.12(-0.71)
Tc	2.17(1.83)	-0.96(-1.26)	-1.14(-1.71)	3.47(3.13)	0.95(0.68)	0.95(0.31)
Ru	3.04(2.71)	0.05(-0.24)	-0.23(-0.87)	3.61(3.06)	2.15(-0.48)	0.51(-0.11)
Rh	1.63(1.22)	-0.04(-0.39)	-1.47(-2.05)	3.41(3.09)	-0.21(-0.59)	-0.01(-0.65)

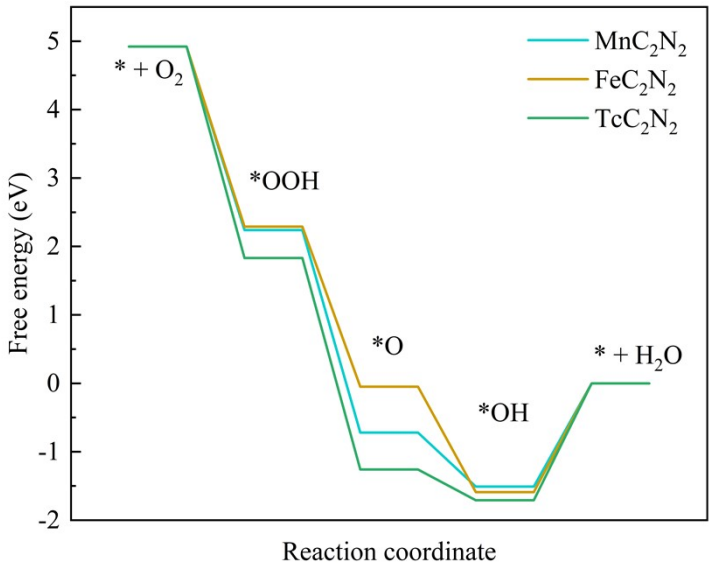


Fig. S4. Free energy diagrams of MnC_2N_2, FeC_2N_2, and TcC_2N_2.