Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Phthalo−carbonitride Nanosheet as Excellent N_2 Reduction Reaction Electrocatalyst: A First−principles Study

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Table S1 The binding energy (E_b, in eV) for transition metal atoms at H1 site of pc−C_3N_2, the cohesive energy (E_c, in eV) for each TM bulk and the ratio E_b/E_c.

TM (H1)	E_b	E_c	E_b/E_c
Ti	-12.34	-5.80	2.13
V	-11.45	-5.60	2.04
Cr	-10.43	-4.01	2.60
Mn	-10.29	-3.48	2.96
Fe	-10.70	-4.63	2.31
Ni	-10.67	-4.88	2.19
Cu	-8.27	-3.65	2.27
Mo	-10.55	-6.78	1.56
Ru	-12.30	-7.97	1.54
W	-12.80	-9.48	1.35

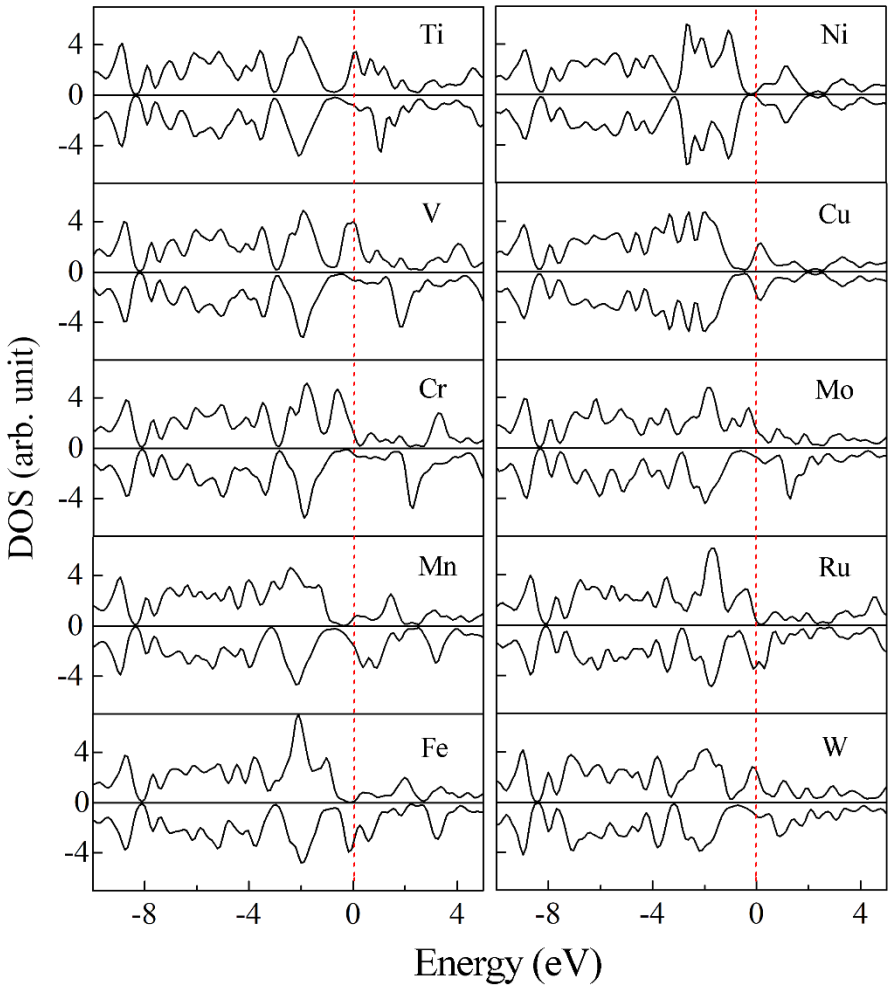

Fig. S1 The DOS of TM@H1 (TM = Ti, V, Cr, Mn, Fe, Ni, Cu, Mo, Ru, and W). The Fermi level is set to zero.

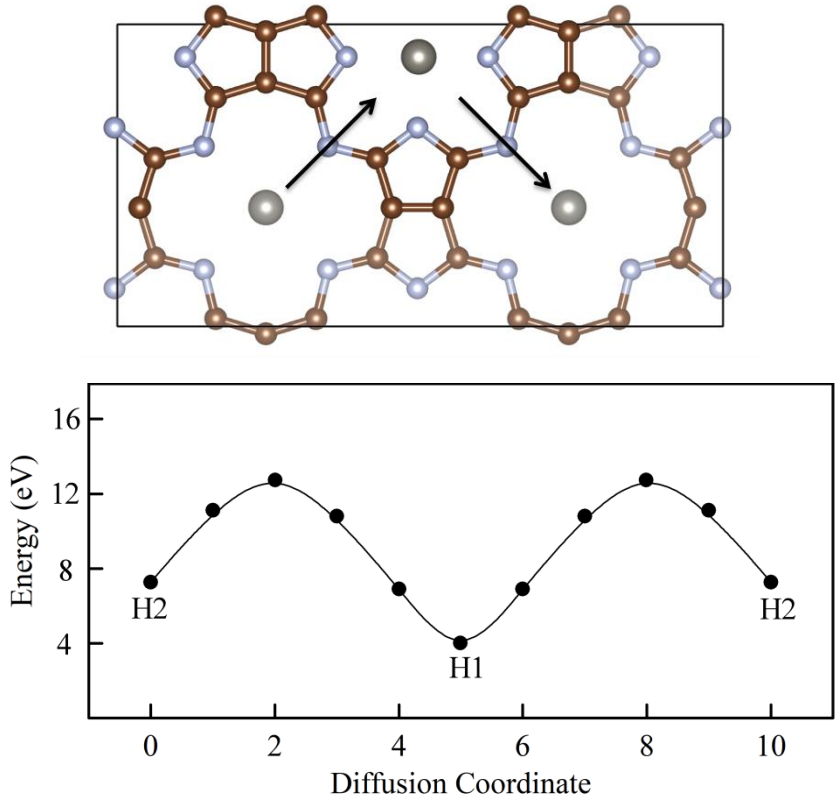

Fig. S2 The minimum energy pathway of W atom moves from one H2 site to another via H1(upper) and the corresponding diffusion barrier (lower).

Table S2. Thermodynamic quantities, in eV (Mild conditions, T= 298.15 K).

	ZPE	**E**	**TΔS**
W*N-N	0.21	–198.31	0.14
***N-NH**	0.48	–202.04	0.18
***N-NH$_2$**	0.83	–205.83	0.18
***N-NH$_3$**	1.03	–210.38	0.29
***NH**	0.37	–194.39	0.08
***NH$_2$**	0.66	–197.92	0.12
***NH$_3$**	1.03	–201.49	0.13
Mo*N-N	0.21	–197.15	0.14
***N-NH**	0.48	–200.69	0.18
***N-NH$_2$**	0.82	–204.23	0.19
***N-NH$_3$**	1.01	–208.86	0.23
***NH**	0.36	–192.63	0.09
***NH$_2$**	0.64	–196.47	0.15
***NH$_3$**	1.02	–200.41	0.19

The atomic coordinates of the systems

W@pc–C_3N_2

C	7.017145732	2.674198924	10.029360056
C	1.015637415	2.674329895	10.019680262
C	2.660395507	1.029713415	10.013420582
C	2.660371114	7.030136128	10.013040304
C	7.017113047	5.385724032	10.028320551
C	1.015604668	5.385544038	10.018639565
C	5.371659526	7.030201492	10.043280125
C	5.371708311	1.029688782	10.043660402
C	7.425941319	4.029912455	10.025080442
C	0.606620894	4.030002452	10.020500422
C	4.015953729	7.439013000	10.034279823
C	4.015896407	0.620844531	10.034459829
N	8.108770522	1.849235032	10.025659800
N	5.695325446	2.351251398	10.036540031
N	2.337351594	2.351431392	10.016399622
N	1.835585631	8.121816689	9.996979833
N	8.108770522	6.210630730	10.023759604
N	2.337392574	5.708499612	10.015640259
N	5.695366425	5.708663510	10.035799742
N	6.196338170	8.121800592	10.052859783
W	4.017279703	4.029879773	10.027600527