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

Supporting Information

Computational Screening of Single Transition Metal Atom Supported on C_2N Monolayer for Electrochemical Ammonia Synthesis

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Table S1. The computed adsorption energy (E_{ads}, eV), distance (d, Å), and charge transfer (Q, $|e|$) of N_2 adsorption on various TM@C_2N monolayers.

TM@C_2N	E_{ads}	d_{TM-N}	d_{N-N}
Sc	-0.56	2.23	1.12
Ti	-0.89	2.04	1.12
V	-0.96	2.00	1.12
Cr	-0.29	1.87	1.13
Mn	-0.46	2.18	1.11
Fe	-1.00	1.91	1.12
Co	-0.93	1.85	1.12
Ni	-0.75	1.87	1.12
Cu	-0.79	1.85	1.12
Zn	-0.51	2.11	1.11
Ru	-0.93	1.92	1.13
Rh	-0.58	2.02	1.12
Pd	-0.29	2.11	1.11
Ag	-0.18	2.74	1.11
Mo	-1.05	1.96	1.14

Table S2. (a) The computed total electronic energies (E, a.u.) of TM@C_2N by considering different formal spin moments (μ_f, μ_B) and the adopted energies in the present work.

	High Spin (E/μ)	Low Spin (E/μ)	Adopted Energies
V@C_2N	-3227.193954/3	-3227.192924/1	-3227.193954
Cr@C_2N	-3244.306176/4	-3244.305082/0	-3244.306176
Mn@C_2N	-3262.864136/5	-3262.864136/1	-3262.864136
Fe@C_2N	-3284.264700/4	-3284.260108/0	-3284.264700
Co@C_2N	-3307.865108/3	-3307.865108/1	-3307.865108
Ni@C_2N	-3334.535923/2	-3334.523759/0	-3334.535923
Mo@C_2N	-3236.526167/4	-3236.500334/0	-3236.526167
Ru@C_2N	-3266.966990/4	-3266.964720/0	-3266.966990
Pd@C_2N	-3304.368651/2	-3304.364825/0	-3304.368651

(b) The computed total electronic energies (E, a.u.) of various NRR species on Mo@C_2N by considering different formal spin moments (μ_f, μ_B) and the adopted energies in the present work.

	High Spin (E/μ)	Low Spin (E/μ)	Adopted Energies
N_2^*	-3346.014752/4	-3346.009458/0	-3346.014752
N_2H^*	-3346.587326/4	-3346.581729/0	-3346.587326
N-NH_2^*	-3347.194220/4	-3347.188472/0	-3347.194220
NH-NH^*	-3347.169023/4	-3347.161458/0	-3347.169023
N^*	-3291.277093/4	-3291.273171/0	-3291.277093
NH-NH_2^*	-3347.788147/4	-3347.782180/0	-3347.788147
NH^*	-3291.871334/4	-3291.870881/0	-3291.871334
NH_2-NH_2^*	-3348.391497/4	-3348.381691/0	-3348.391497
NH_2^*	-3292.4831139/4	-3292.481093/0	-3292.4831139

Table S3. The computed charge transfer (Q, $|e|$), magnetic moment (μ, μ_B), distance (d, Å), and binding energy ($E_{binding}$, eV) of various single TM atoms on C_2N monolayer.

Atom	Q	μ_{tot}/μ_{TM}	$d_{TM\text{-}N}$	$E_{binding}$
Sc	0.93	0.00/0.00	2.28	-7.85
Ti	0.75	1.22/1.58	2.23	-7.17
V	0.57	2.84/3.00	2.11	-6.20
Cr	0.68	3.47/3.85	2.09	-4.83
Mn	0.66	4.58/4.67	2.24	-4.74
Fe	0.49	3.40/3.42	2.15	-4.63
Co	0.38	1.81/1.89	2.00	-4.31
Ni	0.29	1.08/1.19	1.98	-4.47
Cu	0.40	0.00/0.00	2.09	-3.39
Zn	0.68	0.00/0.00	2.09	-1.58
Mo	0.65	2.94/3.36	2.15	-5.42
Rh	0.27	0.00/0.00	2.00	-4.68
Ru	0.41	1.12/1.18	2.02	-5.56
Pd	0.40	0.76/1.02	2.20	-3.28
Ag	0.34	0.00/0.00	2.77	-3.12

Table S4. The computed magnetic moment (μ, μ_B) of various NRR intermediates adsorbed on Mo@C_2N monolayer.

	Total spin moment	Spin moment on Mo	Spin moment on NRR species
N_2^*	1.09	0.98	0.10
N_2H^*	0.98	0.95	-0.12
$N\text{-}NH_2^*$	1.09	1.01	-0.07
$NH\text{-}NH^*$	1.39	1.13	-0.07
N^*	0.87	0.86	-0.09
$NH\text{-}NH_2^*$	1.26	1.15	-0.15
$NH_2\text{-}NH_2^*$	0.92	0.66	-0.11
NH^*	0.00	0.00	0.00
NH_2^*	1.43	1.27	-0.05