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Tantalum based single, double and triple atom catalysts supported on g-C_2N monolayer for effective nitrogen reduction reaction: A comparative DFT investigation

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Table S1: Zero-point and entropic corrections to the free energy of the gas phase and the adsorbed species along the most favourable reaction pathways

Molecule	**E (eV)**	**E_{ZPE} (eV)**	**TS (eV)**	**G (eV)**
H_2	-6.76565715	0.268608	0.4019062	-6.89895535
N_2	-16.62627336	0.149570	0.59182775	-17.06853111
NH_3	-19.54133424	0.909892	0.5951074	-19.22654964
$Ta_1@C_2N$	-639.89016231	0.020942	0.1270119	-639.99623221
$Ta_2@C_2N$	-650.47450021	0.054160	0.2218236	-650.64216381
$Ta_3@C_2N$	-659.63409924	0.073146	0.35151885	-659.91247209
$Ta_1@C_2N$ (Alternate Pathway)				
Step	**E (eV)**	**E_{ZPE} (eV)**	**TS (eV)**	**G (eV)**
$*N_2$	-657.98101494	0.206141	0.15861580	-657.93348974
*NNH	-660.90022764	0.474612	0.16994550	-660.59556114
*NHNH	-663.92654180	0.807607	0.20304015	-663.32197495
$*NHNH_2$	-668.26116294	1.140419	0.20005865	-667.32080259
$*NH_2NH_2$	-671.40667105	1.472140	0.16338620	-670.09791725
$*NH_2$	-657.69660671	0.670640	0.11389330	-657.13986001
$*NH_3$	-660.65714854	0.795866	0.17710110	-660.03838364
$Ta_2@C_2N$ (Alternate Pathway)				
Step	**E (eV)**	**E_{ZPE} (eV)**	**TS (eV)**	**G (eV)**
$*N_2$	-668.45556460	0.260282	0.38580610	-668.58108870
*NNH	-671.22341567	0.531767	0.399819	-671.09146767
*NHNH	-674.82272470	0.863456	0.43321195	-674.39248065
$*NHNH_2$	-679.67905618	1.175413	0.46272880	-678.96637198
$*NH_2NH_2$	-682.57893775	1.524352	0.42933600	-681.48392175
$*NH_2$	-668.48864741	0.766783	0.29755370	-668.01941811
$*NH_3$	-671.73134864	1.069794	0.41204330	-671.07359794
$Ta_3@C_2N$ (Distal Pathway)				
Step	**E (eV)**	**E_{ZPE} (eV)**	**TS (eV)**	**G (eV)**
$*N_2$	-677.68877668	0.284210	0.48509005	-677.88965673
*NNH	-681.32536538	0.564396	0.48747525	-681.24844463
$*NNH_2$	-685.69525532	0.895677	0.49850680	-685.29808512

*N	-671.91985167	0.198271	0.32110755	-671.84441722
*NH	-674.98766614	0.478719	0.37209120	-674.88103834
*NH_2	-677.90478109	0.747179	0.4588528	-677.61645494
*NH_3	-681.15011801	1.093518	0.49850680	-680.55510681

The calculated free energies used for obtaining the free energy pathways for $Ta_1@C_2N$, $Ta_2@C_2N$ and $Ta_3@C_2N$ are -639.99623221, -650.64216381 and -659.91247209 eV, respectively.

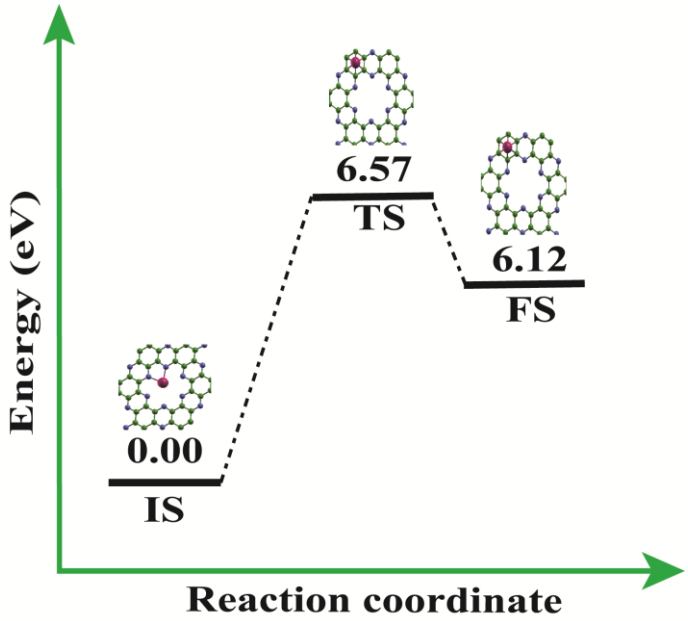

Fig. S1: Diffusion energy barrier of Ta atom from the cavity of g-C_2N to the hexagonal ring.

Table S2: The integrated projected density of states (IDOS) near Fermi level (-2.0 to 0.0 eV) on clean catalysts.

System	Spin	IPDOS (-2.0 to 0.0 eV)
$Ta_1@C2N$	Up	1.73
	Down	-0.23
$Ta_2@C_2N$	Up	2.85
	Down	-1.73
$Ta_3@C_2N$	Up	3.23
	Down	-2.97

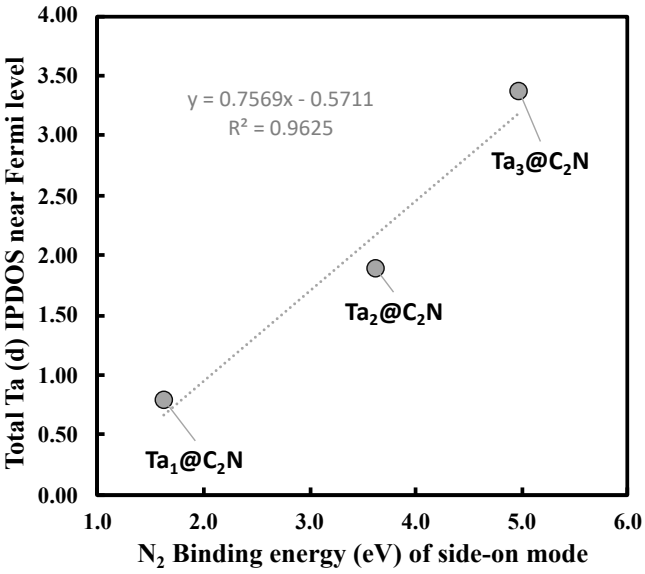

Fig. S2: Total Ta d integrated projected density of states (spin-up + absolute (spin-down)) near Fermi level (-2.0 – 0.0 eV) vs. N_2 binding energies in side-on mode.

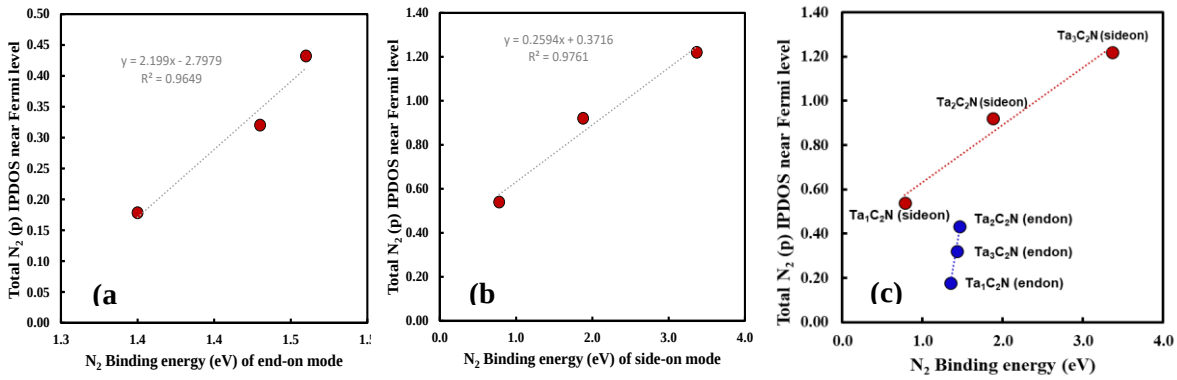

Fig. S3: Total N_2 p-states Integrated projected density of states (spin-up + absolute (spin-down)) near Fermi level (-2.0 – 0.0 eV) vs. N_2 binding energies in (a) side-on mode (b) end-on mode (c) end-on (blue) and side on mode (red).

Table S3: Integrated PDOS (IPDOS) of Ta (d) and N_2 (p) states near Fermi level (in the energy range of -2.0 to 0.0 eV).

System	Element states	Spin	IPODS (-2.0 to 0.0 eV)	
			End-on	Side-on
$Ta_1@C_2N$	Ta (d)	Up	0.97	0.93
		Down	-0.82	-0.7
	N (p)	Up	0.233	0.27
		Down	-0.199	-0.269
$Ta_2@C_2N$	Ta (d)	Up	1.01	1.81
		Down	-0.82	-1.81
	N (p)	Up	0.108	0.46
		Down	-0.07	-0.46
$Ta_3@C_2N$	Ta (d)	Up	3.23	2.49
		Down	-2.85	-2.49
	N (p)	Up	0.17	0.61
			-0.15	-0.61

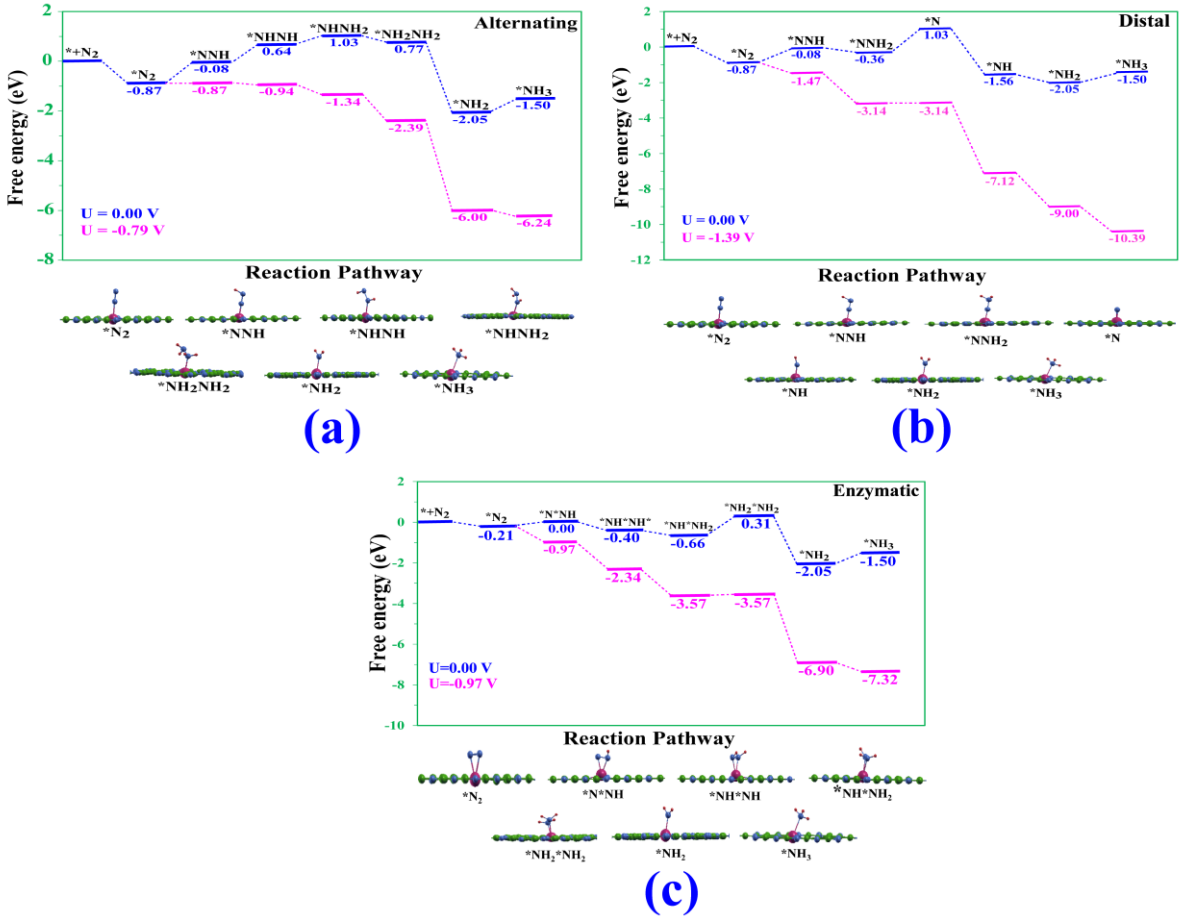

Fig. S4: Detailed nitrogen reduction reaction pathways along the (a) alternate, (b) distal and (c) enzymatic routes on $Ta_1@C_2N$.

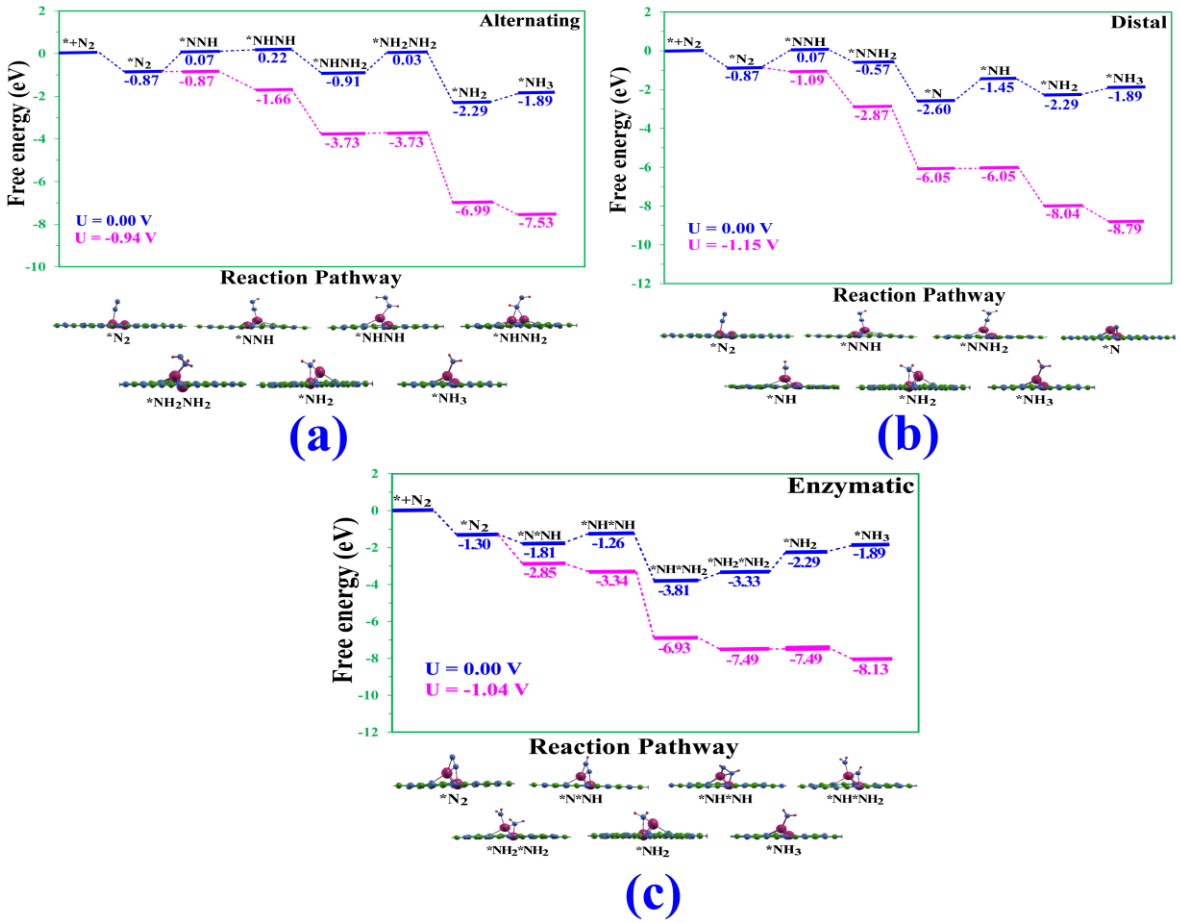

Fig. S5: Detailed nitrogen reduction reaction pathways along the (a) alternate, (b) distal and (c) enzymatic routes on $Ta_2@C_2N$.

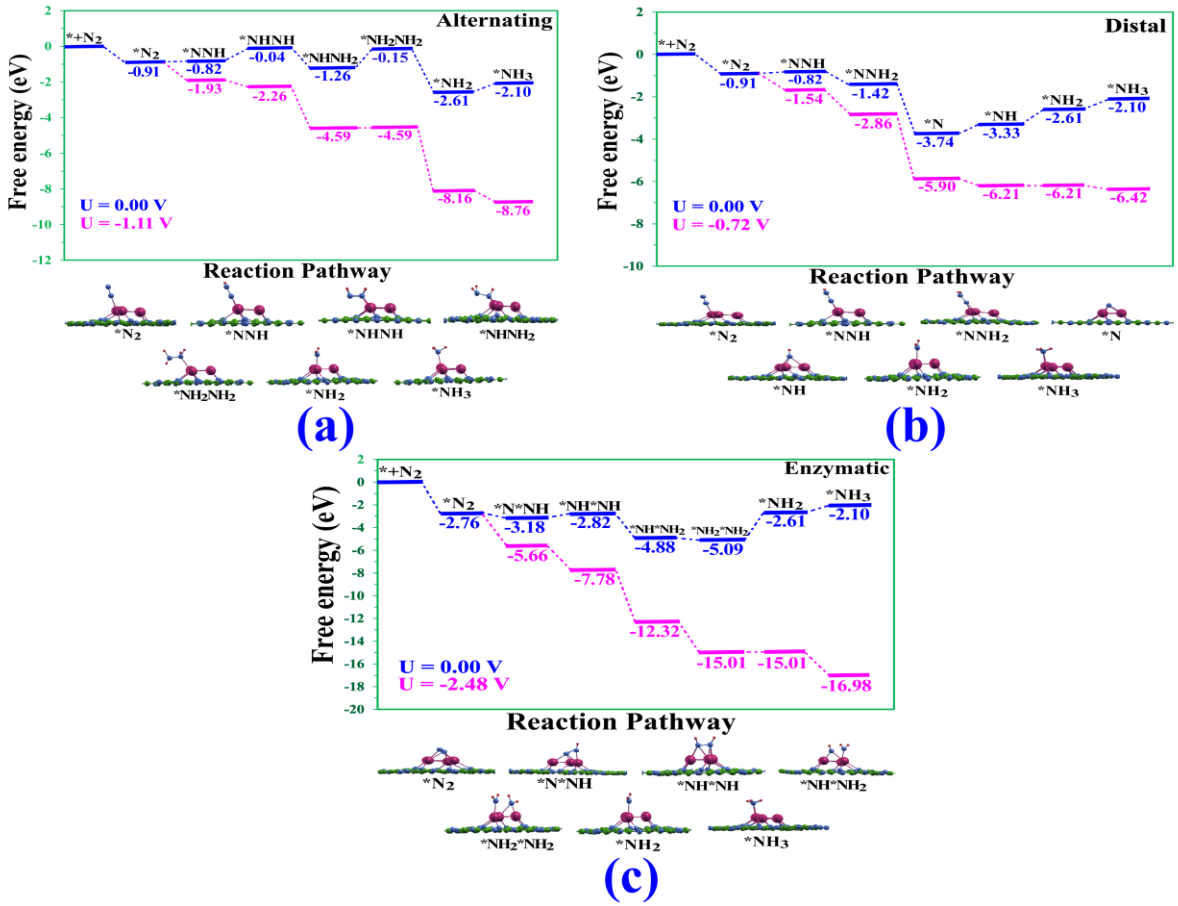

Fig. S6: Detailed nitrogen reduction reaction pathways along the (a) alternate, (b) distal and (c) enzymatic routes on $Ta_3@C_2N$.

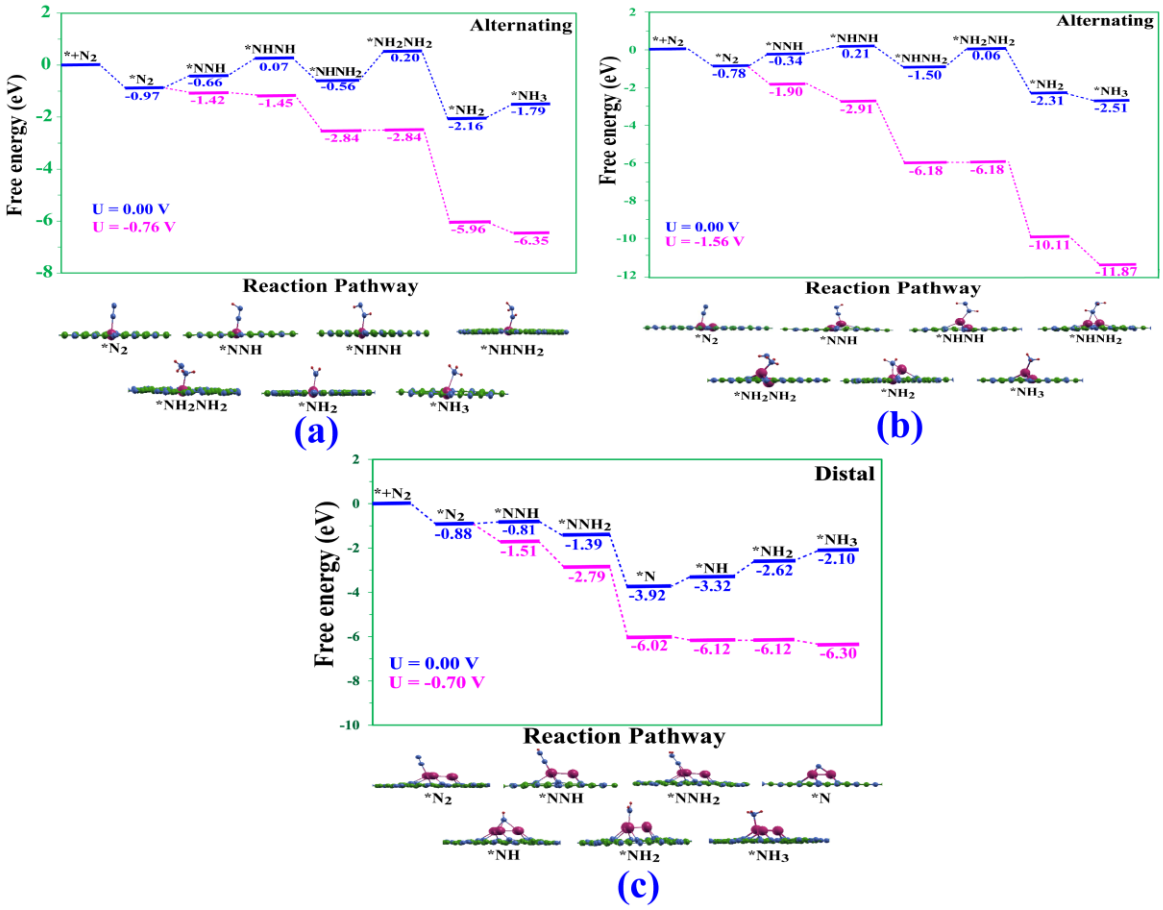

Fig. S7: Most favourable reaction pathway for NRR on the (a) $Ta_1@C_2N$ (b) $Ta_2@C_2N$ and $Ta_3@C_2N$ catalysts with the inclusion of solvent corrections.

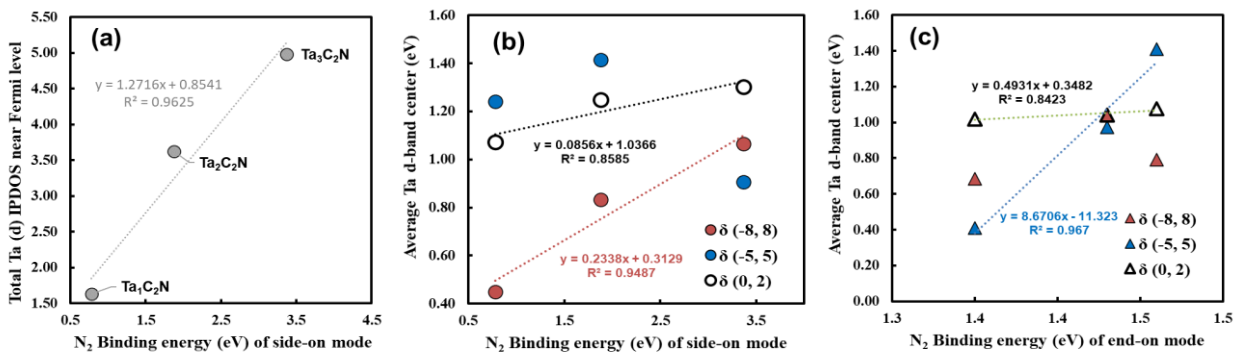

Fig. S8: (a) Total Ta d integrated projected density of states near Fermi level (-2.0 – 0.0 eV) vs. N_2 binding energies in side-on mode. Average d-band centers δ(-8, 8) (energy integration range of -8 to 8 eV), δ(-5, 5) (energy integration range of -5 to 5 eV) and δ(0, 2) (energy integration range of 0 to 2 eV) vs. N_2 binding energies in (b) side-on mode (c) end-on mode.

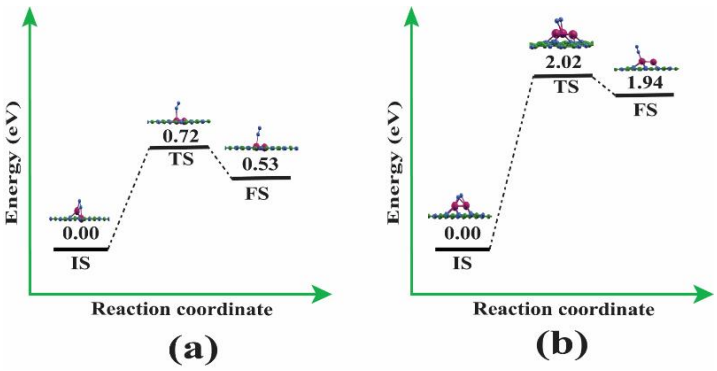

Fig. S9: Activation barriers for side-on to end-on transition for N_2 adsorption on (a) $Ta_2@C_2N$ and (b) $Ta_3@C_2N$ catalysts.

Coordinates of the adsorbed species along the most favorable pathways of NRR on $Ta_1@C_2N$, $Ta_2@C_2N$ and $Ta_3@C_2N$ catalysts

$Ta_1@C_2N$-Alternating pathway

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1.00000000000000
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-8.3299999237000009 14.4279830949000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000
N C Ta
26 48 1
Direct
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0.0000000000000000 0.0000000000000000 15.0000000000000000
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$Ta_2@C_2N$-Alternating pathway

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Direct

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N C Ta H
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