

Fig.S1 Density of states (DOS) of the TM@g-BC₃N₄ system and the Fermi level E_f is set to 0 eV.

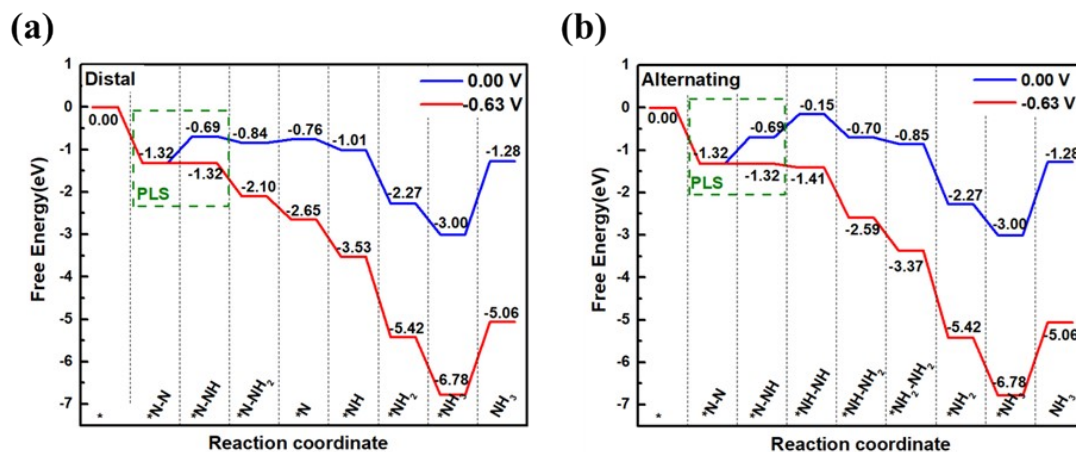


Fig. S2 The NRR reaction free energy diagram of Fe@g-C₃N₄ through (a) distal mechanism and (b) alternating mechanism.

POSCAR-g-BC3N4

1. 0

14. 3542003632	0. 0000000000	0. 0000000000
7. 1774726155	12. 4301933552	0. 0000000000
0. 0000000000	0. 0000000000	20. 0000000000

C	B	N
26	1	36

Direct

0. 058830000	0. 067340001	0. 466600001
0. 058830000	0. 224199995	0. 466600001
0. 215690002	0. 067350000	0. 466600001
0. 392159998	0. 067340001	0. 466600001
0. 392159998	0. 224199995	0. 466600001
0. 549019992	0. 067350000	0. 466600001
0. 725489974	0. 067340001	0. 466600001
0. 725489974	0. 224199995	0. 466600001
0. 882350028	0. 067340001	0. 466600001
0. 058830000	0. 400669992	0. 466600001
0. 058830000	0. 557529986	0. 466600001
0. 215690002	0. 400680006	0. 466600001
0. 392159998	0. 400669992	0. 466600001
0. 392159998	0. 557529986	0. 466600001
0. 725489974	0. 400669992	0. 466600001
0. 725489974	0. 557529986	0. 466600001
0. 882350028	0. 400680006	0. 466600001
0. 058830000	0. 734000027	0. 466600001
0. 058830000	0. 890860021	0. 466600001
0. 215690002	0. 734009981	0. 466600001
0. 392159998	0. 734000027	0. 466600001
0. 392159998	0. 890860021	0. 466600001
0. 549019992	0. 734009981	0. 466600001
0. 725489974	0. 734000027	0. 466600001
0. 725489974	0. 890860021	0. 466600001
0. 882350028	0. 734009981	0. 466600001
0. 549019992	0. 400680006	0. 466600001
0. 000000000	0. 008510000	0. 466600001
0. 002320000	0. 174009994	0. 466600001
0. 165500000	0. 010840000	0. 466600001
0. 165500000	0. 174009994	0. 466600001
0. 333330005	0. 008510000	0. 466600001
0. 335669994	0. 174009994	0. 466600001
0. 498829991	0. 010840000	0. 466600001
0. 498829991	0. 174009994	0. 466600001
0. 666670024	0. 008510000	0. 466600001

0.669000030	0.174009994	0.466600001
0.832159996	0.010840000	0.466600001
0.832159996	0.174009994	0.466600001
0.000000000	0.341839999	0.466600001
0.002320000	0.507350028	0.466600001
0.165509999	0.344170004	0.466600001
0.165500000	0.507350028	0.466600001
0.333330005	0.341839999	0.466600001
0.335669994	0.507350028	0.466600001
0.498840004	0.344170004	0.466600001
0.498829991	0.507350028	0.466600001
0.666670024	0.341839999	0.466600001
0.669000030	0.507350028	0.466600001
0.832159996	0.344170004	0.466600001
0.832159996	0.507350028	0.466600001
0.000000000	0.675180018	0.466600001
0.002320000	0.840680003	0.466600001
0.165509999	0.677510023	0.466600001
0.165500000	0.840680003	0.466600001
0.333330005	0.675180018	0.466600001
0.335660011	0.840680003	0.466600001
0.498840004	0.677510023	0.466600001
0.498829991	0.840680003	0.466600001
0.666670024	0.675180018	0.466600001
0.668990016	0.840680003	0.466600001
0.832170010	0.677510023	0.466600001
0.832159996	0.840680003	0.466600001

POSCAR-Fe@g-BC3N4

1. 0

14. 3542003632	0. 0000000000	0. 0000000000
7. 1774726155	12. 4301933552	0. 0000000000
0. 0000000000	0. 0000000000	20. 0000000000

C	B	N	Fe
26	1	36	1

Direct

0. 060059998	0. 066509999	0. 466600001
0. 060040001	0. 223820001	0. 466600001
0. 216820002	0. 066780001	0. 466600001
0. 392269999	0. 067649998	0. 466600001
0. 389889985	0. 226390004	0. 466600001
0. 549430013	0. 069069996	0. 466600001
0. 726040006	0. 068329997	0. 466600001
0. 730589986	0. 223289996	0. 466600001
0. 884880006	0. 065109998	0. 466600001
0. 058430001	0. 400900006	0. 466600001
0. 057130001	0. 558499992	0. 466600001
0. 214399993	0. 401450008	0. 466600001
0. 389030010	0. 401980013	0. 466600001
0. 389030010	0. 559300005	0. 466600001
0. 730599999	0. 396429986	0. 466600001
0. 726010025	0. 555980027	0. 466600001
0. 884850025	0. 400389999	0. 466600001
0. 057140000	0. 734770000	0. 466600001
0. 058470000	0. 891059995	0. 466600001
0. 214420006	0. 734499991	0. 466600001
0. 389910012	0. 734080017	0. 466600001
0. 392289996	0. 890450001	0. 466600001
0. 549430013	0. 731850028	0. 466600001
0. 724200010	0. 734380007	0. 466600001
0. 724200010	0. 891799986	0. 466600001
0. 881179988	0. 734610021	0. 466600001
0. 555750012	0. 397269994	0. 466600001
0. 001330000	0. 007330000	0. 466600001
0. 004140000	0. 173120007	0. 466600001
0. 166710004	0. 010230000	0. 466600001
0. 166690007	0. 173449993	0. 466600001
0. 334380001	0. 008000000	0. 466600001
0. 335229993	0. 174250007	0. 466600001
0. 499049991	0. 012310000	0. 466600001
0. 497099996	0. 176840007	0. 466600001
0. 666010022	0. 010160000	0. 466600001

0.671190023	0.175070003	0.466600001
0.832650006	0.010410000	0.466600001
0.836939991	0.171049997	0.466600001
0.001300000	0.341740012	0.466600001
0.001260000	0.507700026	0.466600001
0.164810002	0.344559997	0.466600001
0.163619995	0.508360028	0.466600001
0.330399990	0.342999995	0.466600001
0.331730008	0.509289980	0.466600001
0.493880004	0.345620006	0.466600001
0.493889987	0.510779977	0.466600001
0.675119996	0.337590009	0.466600001
0.671180010	0.504059970	0.466600001
0.836939991	0.342350006	0.466600001
0.832620025	0.507300019	0.466600001
0.998310030	0.676050007	0.466600001
0.001300000	0.841440022	0.466600001
0.163640007	0.678380013	0.466600001
0.164849997	0.840990007	0.466600001
0.330419987	0.676940024	0.466600001
0.335249990	0.840879977	0.466600001
0.497119993	0.676400006	0.466600001
0.499060005	0.838989973	0.466600001
0.666000009	0.674179971	0.466600001
0.667859972	0.841260016	0.466600001
0.830780029	0.678200006	0.466600001
0.830770016	0.841409981	0.466600001
0.556869984	0.562240005	0.526000023