Supplementary Information

Tuning surface curvature in B and N co-doped CNT derived Fe, Ru and Ir catalysts for electrochemical hydrogenation of N_2 to NH_3

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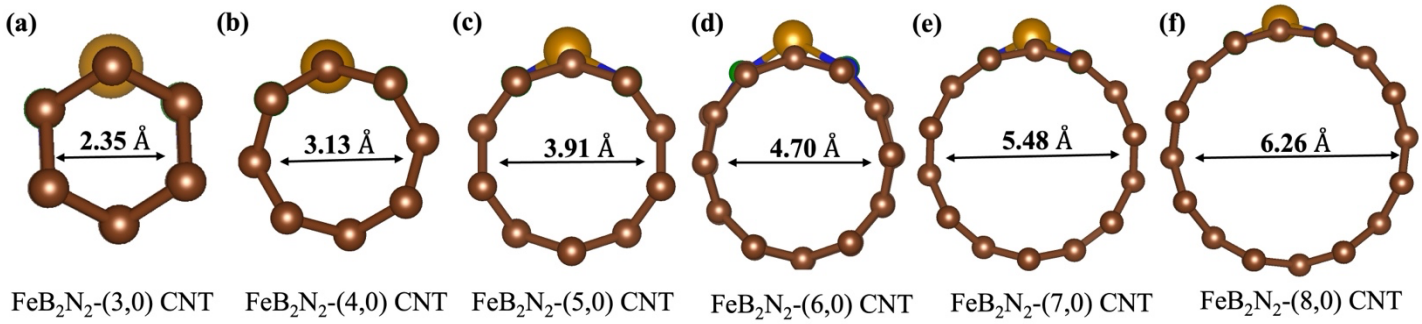

Figure S1. The structural configuration of the FeB_2N_2-(n,0) CNT, where n=3-8 with labelled curvature.

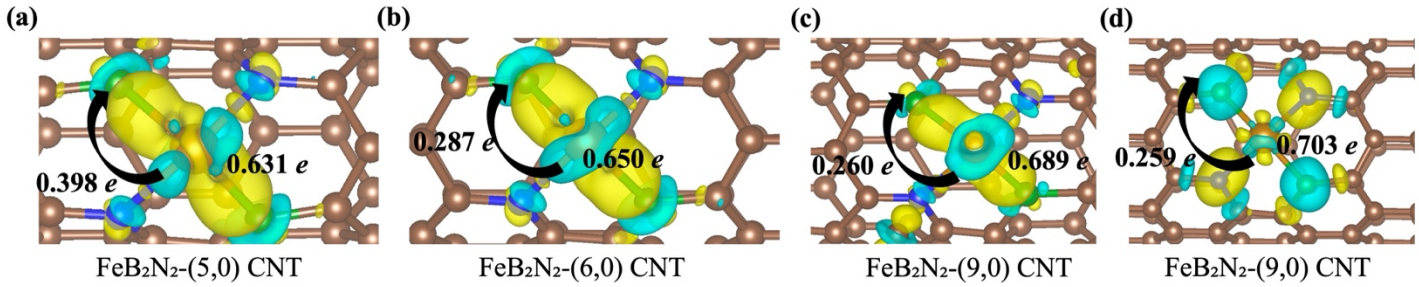

Figure S2. The charge depletion of (a) FeB_2N_2-(5,0) CNT, (b) FeB_2N_2-(6,0) CNT, (c) FeB_2N_2-(7,0) CNT and (d) FeB_2N_2-(8,0) CNT is represented by the cyan region, and accumulation is represented by the yellow region with an isosurface value of 0.004 $e/Å^3$.

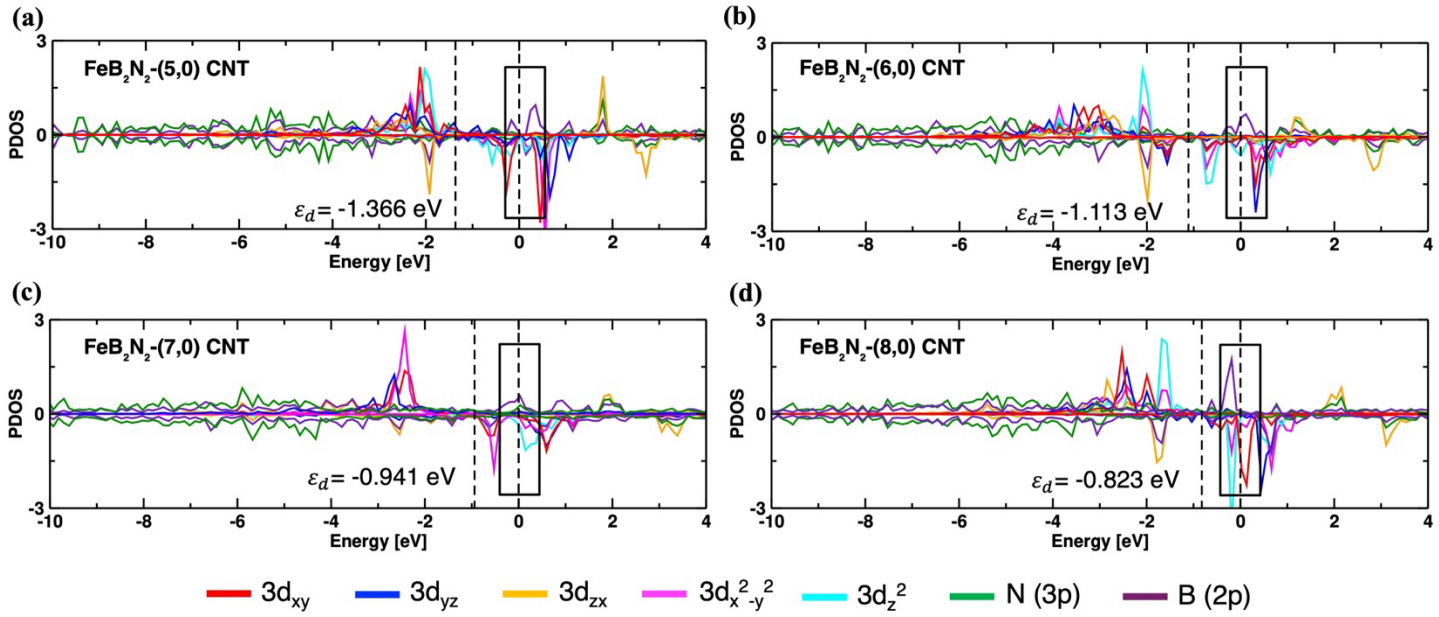

Figure S3. The projected density of states (PDOS) of (a) FeB_2N_2-(5,0) CNT, (b) FeB_2N_2-(6,0) CNT, (c) FeB_2N_2-(7,0) CNT and (d) FeB_2N_2-(8,0) CNT with their respective d-band centre.

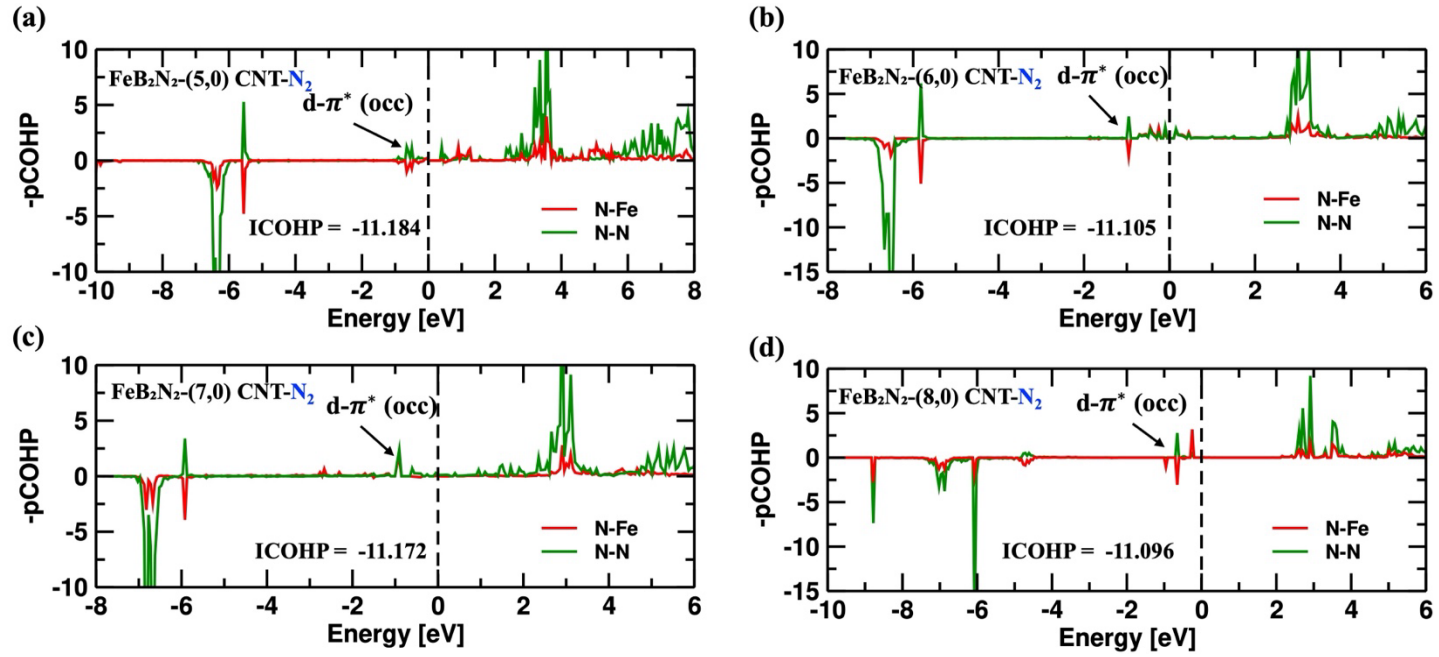

Figure S4. The pCOHP plot of (a) FeB_2N_2-(5,0) CNT, (b) FeB_2N_2-(6,0) CNT, (c) FeB_2N_2-(7,0) CNT and (d) FeB_2N_2-(8,0) CNT with the corresponding ICOHP value of N_2.

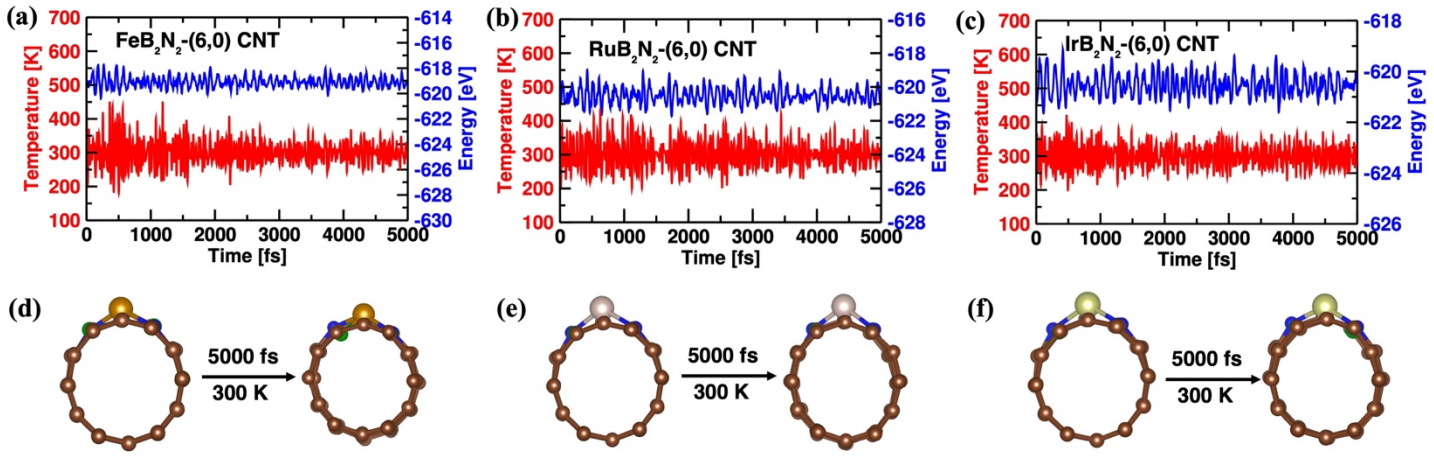

Figure S5. The change in temperature and energy during AIMD simulation at 300K for (a) FeB_2N_2-(6,0) CNT (b) Ru B_2N_2-(6,0) CNT and (c) IrB_2N_2-(6,0) CNT with their corresponding structure change (d), (e) and (f), respectively.

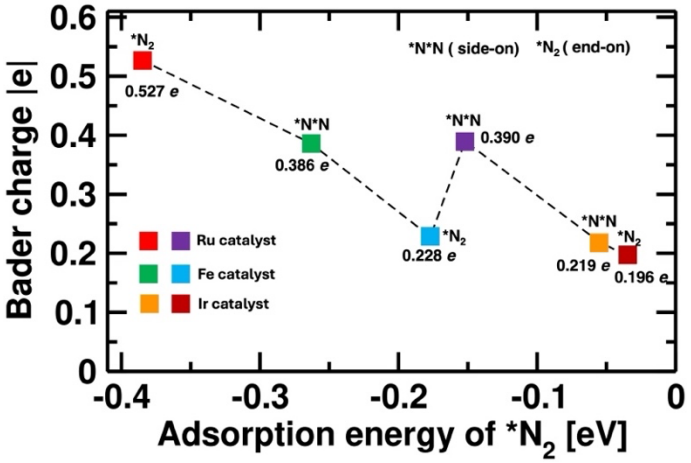

Figure S6. The relationship between the charge transfer from metal catalyst to the $*N_2$ in both end-on ($*N_2$) and side-on mode (*N*N).

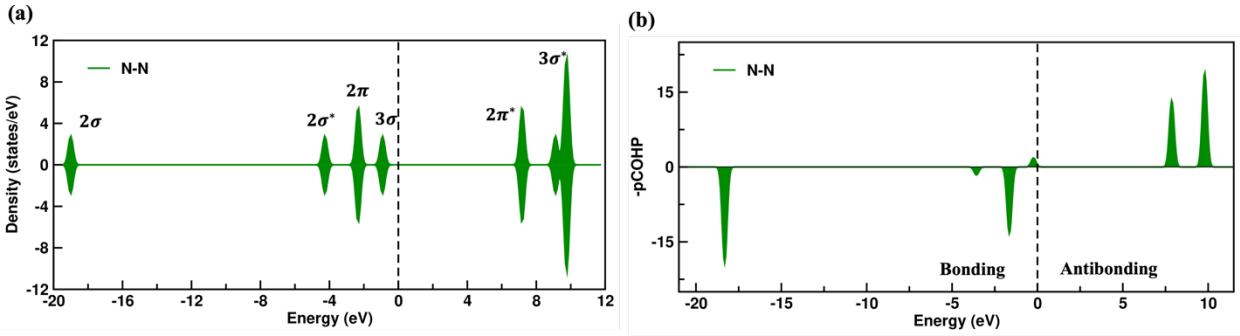

Figure S7. (a) The PDOS of free N_2 (b) The pCOHP of free N_2 molecule.

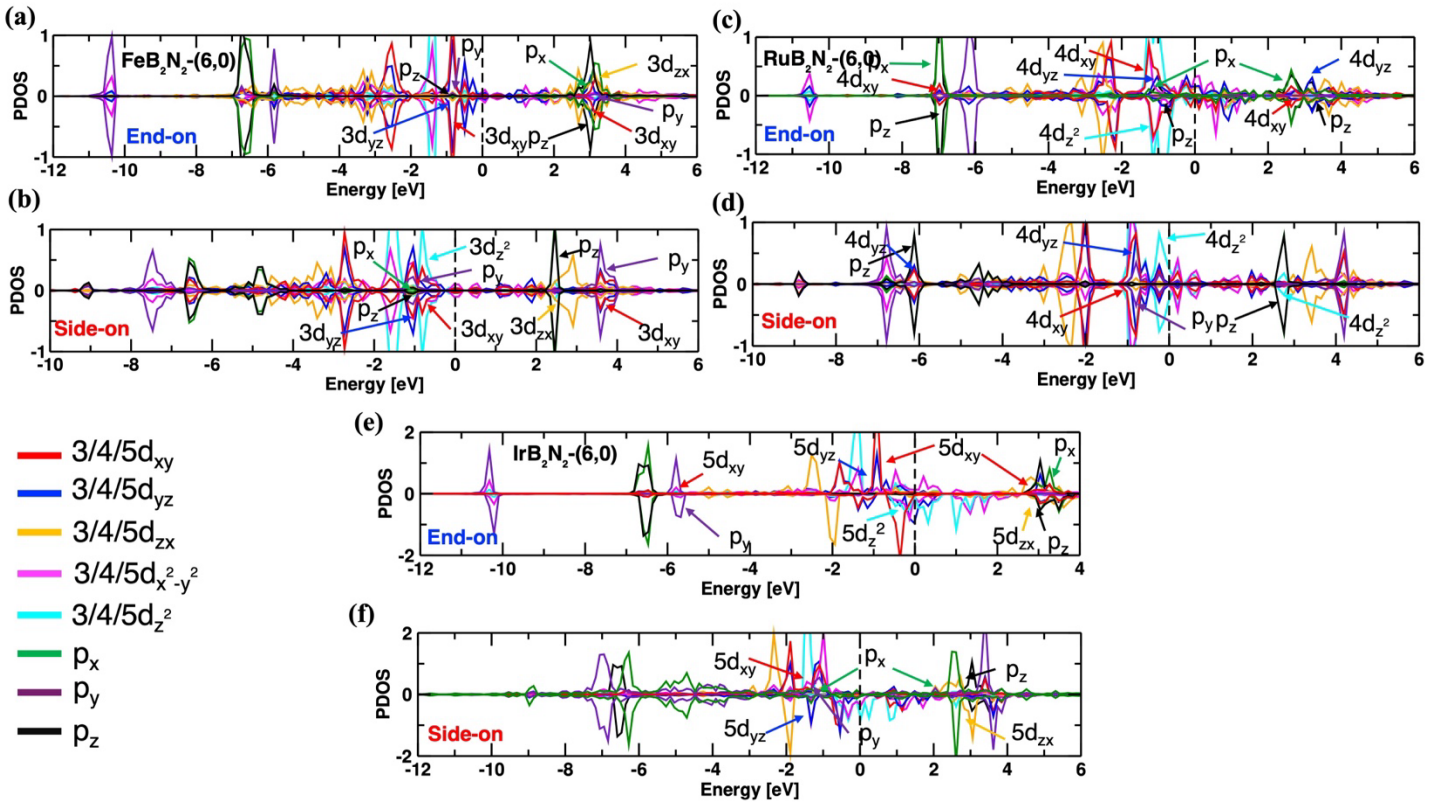

Figure S8. The orbital analysis of the N_2 with the metal centre (a) End-on $*N_2$ adsorption, (b) Side-on $*N_2$ adsorption on FeB_2N_2-(6,0) CNT. (c) End-on $*N_2$ adsorption, (d) Side-on $*N_2$ adsorption on RuB_2N_2-(6,0) CNT. (e) End-on $*N_2$ adsorption, (f) Side-on $*N_2$ adsorption on IrB_2N_2-(6,0) CNT.

Table S1. The formula used for formation energy calculation for the NRR intermediates.

S. No	intermediates	Formation Energy
1	*N2	$\Delta G(*N_2) = G(*N_2) - [G(slab) + G(N_2(g))]$
2	**N2	$\Delta G(**N_2) = G(**N_2) - [G(slab) + G(N_2(g))]$
3	*NNH	$\Delta G(*NNH) = G(*NNH) - [G(slab) + G(N_2(g)) + G(H+ + e-)]$
4	*N*NH	$\Delta G(*N*NH) = G(*N*NH) - [G(slab) + G(N_2(g)) + G(H+ + e -)]$
5	*NNH$_2$	$\Delta G(*NNH_2) = G(*NNH_2) - [G(slab) + G(N_2(g)) + 2G(H+ + e-)]$
6	*NHNH	$\Delta G(*NHNH) = G(*NHNH) - [G(slab) + G(N_2(g)) + 2G(H+ + e -)]$
7	*NH*NH	$\Delta G(*NH*NH) = G(*NH*NH) - [G(slab) + G(N_2(g)) + 2G(H+ + e -)]$
8	*NHNH$_2$	$\Delta G(*NHNH_2) = G(*NHNH_2) - [G(slab) + G(N_2(g)) + 3G(H+ + e-)]$
9	*NH*NH$_2$	$\Delta G(*NH*NH_2) = G(*NH*NH_2) - [G(slab) + G(N_2(g)) + 3G(H+ + e-)]$
10	*N	$\Delta G(*N) = G(*N) - [G(slab) + 1/2G(N_2(g))]$
11	*NH	$\Delta G(*NH) = G(*NH) - [G(slab) + 1/2G(N_2(g)) + G(H+ + e -)]$
12	*NH$_2$NH$_2$	$\Delta G(*NH_2NH_2) = G(*NH_2NH_2) - [G(slab) + G(N_2(g)) + 4G(H+ + e-)]$
13	*NH$_2$*NH$_2$	$\Delta G(*NH_2*NH2) = G(*NH_2*NH2) - [G(slab) + G(N_2(g)) + 4G(H+ + e-)]$
14	*NH$_2$	$\Delta G(*NH_2) = G(*NH_2) - [G(slab) + 1/2G(N_2(g)) + 2G(H+ + e -)]$
15	*NH$_3$	$\Delta G(*NH_3) = G(*NH_3) - [G(slab) + 1/2G(N_2(g)) + 3G(H+ + e -)]$
16	*H	$\Delta G(*H) = G(*H) - [G(slab) + 1/2G(H2(g))]$

Table S2. Calculated total energies (E) and thermodynamic quantities for gas phase species at T = 298.15 K, P = 1 bar) consistent with experimental thermodynamic quantity (TS_{exp}).

Species	**Energy**	**ZPE**	**TS**	**G**	**TS_{exp}**
N_2 (g)	-16.634	0.148	0.592	-17.078	0.590
H_2 (g)	-6.76	0.269	0.403	-6.894	0.410
NH_3 (g)	-19.539	0.911	0.595	-19.223	0.600

Table S3. The Gibbs free energy changes of each intermediate step involved in the FeB_2N_2-(6, 0) CNTs three pathways.

Distal	$*N_2$	*NNH	$*NNH_2$	*N	*NH	$*NH_2$	$*NH_3$
ΔG (eV)	-0.177	0.386	0.416	0.174	0.046	-1.018	-1.172
Alternating	$*N_2$	*NNH	*NHNH	$*NHNH_2$	$*NH_2NH_2$	*NH2	$*NH_3$
ΔG (eV)	-0.177	0.386	0.824	0.271	0.397	-1.018	-1.172
Enzymatic	*N*N	*N*NH	*NH*NH	$*NH*NH_2$	$*NH_2*NH_2$	$*NH_2$	$*NH_3$
ΔG (eV)	-0.263	0.288	0.649	0.731	-0.852	-1.018	-1.172

Table S4. The Gibbs free energy changes of each intermediate step involved in the RuB_2N_2-(6, 0) CNTs three pathways.

Distal	$*N_2$	*NNH	$*NNH_2$	$*N--NH_3$	*NH	$*NH_2$	$*NH_3$
ΔG (eV)	-0.385	0.381	0.182	-0.122	-0.312	-0.795	-0.921
Alternating	$*N_2$	*NNH	*NHNH	$*NHNH_2$	$*NHNH_2$	*NH2	$*NH_3$
ΔG (eV)	-0.385	0.381	0.608	0.334	0.771	-0.795	-0.921
Enzymatic	*N*N	*N*NH	*NH*NH	$*NH*NH_2$	$*NH_2*NH_2$	$*NH_2$	$*NH_3$
ΔG (eV)	-0.152	0.312	0.614	-0.019	0.846	-0.795	-0.921

Table S5. The Gibbs free energy changes of each intermediate step involved in the IrB_2N_2-(6, 0) CNTs three pathways.

Distal	$*N_2$	*NNH	$*NNH_2$	$*N--NH_3$	*NH	$*NH_2$	$*NH_3$
ΔG (eV)	-0.035	0.810	0.748	0.702	0.430	-0.495	-0.578
Alternating	$*N_2$	*NNH	*NHNH	$*NHNH_2$	$*NHNH_2$	*NH2	$*NH_3$
ΔG (eV)	-0.035	0.810	1.119	0.800	0.312	-0.495	-0.578
Enzymatic	*N*N	*N*NH	*NH*NH	$*NH*NH_2$	$*NH_2*NH_2$	$*NH_2$	$*NH_3$
ΔG (eV)	-0.055	1.153	0.773	0.572	-1.278	-0.495	-0.578

Table S6. Calculated ΔZPE and TΔS of intermediates on FeB_2N_2-(6, 0) CNT at T= 298.15.

Intermediates	**ΔZPE (eV)**	**TΔS (eV)**
$*N_2$	0.168	0.098
*N*N	0.185	0.161
*NNH	0.481	0.171
*N*NH	0.491	0.138
$*NNH_2$	0.788	0.153
*NHNH	0.813	0.174
*NH*NH	0.773	0.169
*N	0.087	0.063
$*NHNH_2$	1.121	0.174
$*NH*NH_2$	1.025	0.199
*NH	0.324	0.111
$*NH_2NH_2$	1.464	0.186
$*NH_2*NH_2$	1.367	0.212
$*NH_2$	0.649	0.156
$*NH_3$	1.004	0.157
*H (on Metal)	0.000	0.000
*H (on Boron)	0.248	0.04

Table S7. Calculated ΔZPE and TΔS of intermediates on RuB_2N_2-(6, 0) CNT at T= 298.15.

Intermediates	**ΔZPE**	**TΔS**
$*N_2$	0.196	0.178
*N*N	0.187	0.158
*NNH	0.473	0.176

*N*NH	0.490	0.148
*NNH_2	0.794	0.207
*NHNH	0.817	0.150
*NH*NH	0.830	0.168
*N	0.088	0.060
*$NHNH_2$	1.130	0.197
NHNH_2	1.149	0.175
*NH	0.351	0.079
*NH_2NH_2	1.476	0.198
*NH_2*NH_2	1.463	0.172
*NH_2	0.659	0.080
*NH_3	1.020	0.117
*H (on Metal)	0.210	0.009
*H (on Boron)	0.192	0.030

Table S8. Calculated ΔZPE and TΔS of intermediates on IrB_2N_2-(6, 0) CNT at T= 298.15.

Intermediates	**ΔZPE**	**TΔS**
*N_2	0.287	0.028
*N*N	0.187	0.160
*NNH	0.473	0.174
*N*NH	0.448	0.110
*NNH_2	0.783	0.148
*NHNH	0.817	0.150
*NH*NH	0.817	0.153
*N	0.086	0.073
*$NHNH_2$	1.128	0.215
NHNH_2	1.153	0.183
*NH	0.337	0.111
*NH_2NH_2	1.501	0.153
*NH_2*NH_2	1.446	0.223
*NH_2	0.644	0.078
*NH_3	1.000	0.096
*H (on Metal)	0.184	0.040
*H (on Boron)	0.172	0.035

VASP input parameter

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ISPIN = 2
ENCUT = 600
PREC = Accurate
LREAL= .Auto
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SIGMA = 0.05
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EDIFFG = -0.001
NELM = 100
NELMIN = 4
NSW = 1000
IBRION = 2
ISIF = 2
IVDW = 11
LWAVE = .TRUE

Coordinates of the FeB_2N_2-(n,0) CNT, where n=3-8

FeB_2N_2-(8,0) CNT

C	8.149999	4.953500	1.478561
C	8.149999	4.953500	2.898507
C	7.682400	6.082500	3.608480
C	7.682400	6.082500	0.768589
C	6.818400	6.946500	1.478561
C	6.818400	6.946500	2.898507
C	5.689600	7.414000	3.608480
C	5.689600	7.414000	0.768589
C	4.467700	7.414000	1.478561
C	4.467700	7.414000	2.898507
C	3.338900	6.946500	3.608480
C	3.338900	6.946500	0.768589
C	2.474900	6.082500	1.478561
C	2.474900	6.082500	2.898507
C	2.007300	4.953500	3.608480
C	2.007300	4.953500	0.768589
C	2.007300	3.731750	1.478561
C	2.007300	3.731750	2.898507
C	2.474900	2.602750	3.608480
C	2.474900	2.602750	0.768589
C	3.338900	1.738750	1.478561
C	3.338900	1.738750	2.898507
C	4.467700	1.271250	3.608480
C	4.467700	1.271250	0.768589
C	5.689600	1.271250	1.478561
C	5.689600	1.271250	2.898507
C	6.818400	1.738750	3.608480
C	6.818400	1.738750	0.768589
C	7.682400	2.602750	1.478561
C	7.682400	2.602750	2.898507
C	8.149999	3.731750	3.608480
C	8.149999	3.731750	0.768589
C	8.149999	4.953500	5.738525
C	8.149999	4.953500	7.158470
C	7.682400	6.082500	7.868570
C	7.682400	6.082500	5.028551
C	6.818400	6.946500	5.738525
C	6.818400	6.946500	7.158470
C	2.474900	6.082500	5.738525
C	2.474900	6.082500	7.158470
C	2.007300	4.953500	7.868570
C	2.007300	4.953500	5.028551
C	2.007300	3.731750	5.738525
C	2.007300	3.731750	7.158470
C	2.474900	2.602750	7.868570
C	2.474900	2.602750	5.028551
C	3.338900	1.738750	5.738525
C	3.338900	1.738750	7.158470
C	4.467700	1.271250	7.868570
C	4.467700	1.271250	5.028551
C	5.689600	1.271250	5.738525
C	5.689600	1.271250	7.158470
C	6.818400	1.738750	7.868570
C	6.818400	1.738750	5.028551
C	7.682400	2.602750	5.738525
C	7.682400	2.602750	7.158470
C	8.149999	3.731750	7.868570
C	8.149999	3.731750	5.028551

C	8.149999	4.953500	9.998488
C	8.149999	4.953500	11.418560
C	7.682400	6.082500	12.128533
C	7.682400	6.082500	9.288516
C	6.818400	6.946500	9.998488
C	6.818400	6.946500	11.418560
C	5.689600	7.414000	12.128533
C	5.689600	7.414000	9.288516
C	4.467700	7.414000	9.998488
C	4.467700	7.414000	11.418560
C	3.338900	6.946500	12.128533
C	3.338900	6.946500	9.288516
C	2.474900	6.082500	9.998488
C	2.474900	6.082500	11.418560
C	2.007300	4.953500	12.128533
C	2.007300	4.953500	9.288516
C	2.007300	3.731750	9.998488
C	2.007300	3.731750	11.418560
C	2.474900	2.602750	12.128533
C	2.474900	2.602750	9.288516
C	3.338900	1.738750	9.998488
C	3.338900	1.738750	11.418560
C	4.467700	1.271250	12.128533
C	4.467700	1.271250	9.288516
C	5.689600	1.271250	9.998488
C	5.689600	1.271250	11.418560
C	6.818400	1.738750	12.128533
C	6.818400	1.738750	9.288516
C	7.682400	2.602750	9.998488
C	7.682400	2.602750	11.418560
C	8.149999	3.731750	12.128533
C	8.149999	3.731750	9.288516
N	5.689600	7.414000	7.868570
N	3.338900	6.946500	5.028551
B	5.689600	7.414000	5.028551
B	3.338900	6.946500	7.868570
Fe	4.480800	7.593000	6.454954
C	7.682400	6.082500	13.428588
C	5.689600	7.414000	13.428588
C	3.338900	6.946500	13.428588
C	2.007300	4.953500	13.428588
C	2.474900	2.602750	13.428588
C	4.467700	1.271250	13.428588
C	6.818400	1.738750	13.428588
C	8.149999	3.731750	13.428588

FeB_2N_2-(7,0) CNT

C	1.946200	2.901000	11.422832
C	2.015900	2.897000	10.004494
C	1.638300	4.042500	9.271892
C	1.659500	5.261500	11.402060
C	1.729200	5.257500	9.983848
C	2.402900	6.293750	9.303177
C	1.708000	4.038500	7.853681
C	3.324000	6.957750	11.479069
C	3.393700	6.953750	10.060730
C	4.637600	7.099000	9.410586
C	5.686200	6.712500	11.595723
C	5.755900	6.708750	10.177511
C	6.659500	5.852000	9.513432

C 6.967400 4.710750 11.664373
C 7.037100 4.706750 10.246034
C 6.946200 3.491750 9.534205
C 6.729200 5.848000 8.095094
C 6.202800 2.459500 11.633088
C 6.272400 2.455500 10.214876
C 5.281700 1.795500 9.457197
C 7.015800 3.487750 8.115866
C 3.968100 1.654000 11.525680
C 4.037800 1.650000 10.107342
C 2.919500 2.040500 9.340415
C 5.351400 1.791500 8.038857
C 2.989200 2.036500 7.922203
C 2.155200 2.889000 7.167943
C 2.224800 2.885250 5.749731
C 1.847300 4.030500 5.017003
C 1.868500 5.249500 7.147297
C 1.938200 5.245500 5.728959
C 1.917000 4.026500 3.598791
C 2.681600 6.277750 3.629949
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C 5.560400 1.779500 3.784094
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C 2.364200 2.877250 2.913053
C 2.433800 2.873250 1.494841
C 2.056300 4.018500 0.762240
C 2.077500 5.237500 2.892408
C 2.147200 5.233500 1.474069
C 2.820900 6.269750 0.793398
C 3.742000 6.933750 2.969417
C 3.811600 6.929750 1.551078
C 5.055600 7.075250 0.900933
C 6.104200 6.688750 3.086071
C 6.173900 6.684750 1.667732
C 7.077500 5.828250 1.003780
C 7.385400 4.686750 3.154594
C 7.455000 4.682750 1.736382
C 7.364200 3.467750 1.024426
C 6.620800 2.435500 3.123436
C 6.690400 2.431500 1.705097
C 5.699700 1.771500 0.947417
C 4.386100 1.630250 3.015901
C 4.455800 1.626250 1.597689
C 3.337500 2.016500 0.830763
B 2.472600 6.289750 7.884839
B 4.846600 7.087250 5.155822
N 4.707300 7.095000 7.992373

N	2.611900	6.281750	5.048288
Fe	3.551000	7.292000	6.471819
C	2.125900	4.014499	-0.656099
C	2.890600	6.265750	-0.624814
C	5.125200	7.071250	-0.517405
C	7.147200	5.824250	-0.414559
C	7.433800	3.463750	-0.393786
C	5.769300	1.767500	-0.470794
C	3.407100	2.012750	-0.587576

FeB_2N_2-(6,0) CNT

C	6.399266	5.560533	1.193929
C	7.022738	4.482675	3.317979
C	7.050251	4.448678	4.733918
C	4.083085	6.290167	1.195610
C	6.389026	5.574835	2.605741
C	5.335134	6.288401	3.296788
C	2.479546	4.506409	1.171860
C	4.074522	6.302780	2.596882
C	3.014547	5.603640	3.337717
C	3.101690	2.145028	1.158790
C	2.486886	4.488227	2.585419
C	2.529311	3.221153	3.258242
C	2.534290	3.209783	4.652169
C	5.414636	1.444069	1.177478
C	3.108452	2.119824	2.557488
C	4.166697	1.450488	3.279507
C	4.170040	1.441581	4.679976
C	7.054470	3.228787	1.190760
C	5.424719	1.438123	2.570091
C	6.496014	2.096398	3.293975
C	6.498711	2.075256	4.690363
C	7.050492	3.236420	2.598089
C	6.514645	5.548384	5.480002
C	7.020577	4.410779	7.547655
C	7.018973	4.423771	8.940459
C	6.431936	5.509009	6.870610
C	5.398979	6.237704	8.861526
C	2.486273	4.454988	5.329172
C	3.044130	5.679791	8.904284
C	3.116741	2.116650	5.386212
C	2.394607	4.448292	6.719743
C	2.490778	3.227831	7.465393
C	2.497411	3.270506	8.881525
C	5.425509	1.411997	5.401840
C	3.109139	2.122496	6.790084
C	4.164038	1.455655	7.510249
C	4.155076	1.474922	8.906462
C	7.077592	3.182361	5.410460
C	5.424020	1.411712	6.798846
C	6.499788	2.059947	7.521022
C	6.498081	2.070179	8.919479
C	7.072811	3.172661	6.813284
C	6.414542	5.538008	9.614084
C	7.023839	4.468941	11.737006
C	7.015556	4.475311	0.480844
C	4.132481	6.318073	9.602109
C	6.412212	5.558512	11.027634
C	5.373793	6.252915	11.743592

C	5.352713	6.244946	0.481377
C	2.491486	4.532761	9.594878
C	4.131577	6.303348	11.003359
C	3.052545	5.632567	11.718608
C	3.030157	5.628529	0.455757
C	3.103805	2.181829	9.602188
C	2.490292	4.515391	11.005681
C	2.507037	3.266746	11.719238
C	2.503361	3.257362	0.462426
C	5.411516	1.434702	9.629553
C	3.104421	2.172023	11.009591
C	4.154459	1.484832	11.722477
C	4.158852	1.476631	0.452793
C	7.077639	3.181068	9.642499
C	5.417377	1.444242	11.021256
C	6.490798	2.097499	11.747450
C	6.490615	2.107400	0.476923
C	7.070801	3.206269	11.040214
B	5.456840	6.321060	4.767364
B	2.920421	5.647118	7.435168
N	2.925327	5.629479	4.697022
N	5.463139	6.304938	7.502117
Fe	3.985977	6.735616	6.094639
C	7.015556	4.475311	13.146844
C	5.352713	6.244946	13.147377
C	4.158852	1.476631	13.118793
C	6.490615	2.107400	13.142923

FeB_2N_2-(5,0) CNT

C	6.622000	4.152250	1.400576
C	6.622000	4.152250	2.820608
C	5.911000	5.131000	3.530624
C	5.911000	5.131000	0.690560
C	4.760600	5.504750	1.400576
C	4.760600	5.504750	2.820608
C	3.610100	5.131000	3.530624
C	3.610100	5.131000	0.690560
C	2.899100	4.152250	1.400576
C	2.899100	4.152250	2.820608
C	2.899100	2.942750	3.530624
C	2.899100	2.942750	0.690560
C	3.610100	1.964000	1.400576
C	3.610100	1.964000	2.820608
C	4.760600	1.590250	3.530624
C	4.760600	1.590250	0.690560
C	5.911000	1.964000	1.400576
C	5.911000	1.964000	2.820608
C	6.622000	2.942750	3.530624
C	6.622000	2.942750	0.690560
C	6.622000	4.152250	5.660544
C	6.622000	4.152250	7.080576
C	2.899100	4.152250	5.660544
C	2.899100	4.152250	7.080576
C	2.899100	2.942750	7.790592
C	2.899100	2.942750	4.950657
C	3.610100	1.964000	5.660544
C	3.610100	1.964000	7.080576
C	4.760600	1.590250	7.790592
C	4.760600	1.590250	4.950657

C	5.911000	1.964000	5.660544
C	5.911000	1.964000	7.080576
C	6.622000	2.942750	7.790592
C	6.622000	2.942750	4.950657
C	6.622000	4.152250	9.920640
C	6.622000	4.152250	11.340545
C	5.911000	5.131000	12.050560
C	5.911000	5.131000	9.210624
C	4.760600	5.504750	9.920640
C	4.760600	5.504750	11.340545
C	3.610100	5.131000	12.050560
C	3.610100	5.131000	9.210624
C	2.899100	4.152250	9.920640
C	2.899100	4.152250	11.340545
C	2.899100	2.942750	12.050560
C	2.899100	2.942750	9.210624
C	3.610100	1.964000	9.920640
C	3.610100	1.964000	11.340545
C	4.760600	1.590250	12.050560
C	4.760600	1.590250	9.210624
C	5.911000	1.964000	9.920640
C	5.911000	1.964000	11.340545
C	6.622000	2.942750	12.050560
C	6.622000	2.942750	9.210624
B	5.911000	5.131000	4.950652
B	3.610100	5.131000	7.790592
N	5.911000	5.131000	7.790592
N	3.610100	5.131000	4.950652
Fe	4.674000	5.768250	6.515328
C	5.911000	5.131000	13.490560
C	3.610100	5.131000	13.490560
C	2.899100	2.942750	13.490560
C	4.760600	1.590250	13.490560
C	6.622000	2.942750	13.490560

FeB_2N_2-(4,0) CNT

C	2.572774	4.047503	0.482445
C	1.415261	4.357655	1.192502
C	2.572774	4.047503	3.322417
C	0.377405	3.758448	0.482445
C	0.067279	2.600881	1.192502
C	1.415261	4.357655	2.612488
C	0.377405	3.758448	3.322417
C	0.666476	1.563042	0.482445
C	1.823989	1.252891	1.192502
C	0.067279	2.600881	2.612488
C	0.666476	1.563042	3.322417
C	2.861845	1.852097	0.482445
C	3.171971	3.009665	1.192502
C	1.823989	1.252891	2.612488
C	2.861845	1.852097	3.322417
C	3.171971	3.009665	2.612488
B	2.572774	4.047503	4.742402
Fe	1.415261	4.357655	6.120000
N	2.572774	4.047503	7.582502
N	0.377405	3.758448	4.742402
C	0.067279	2.600881	5.452459
B	0.377405	3.758448	7.582502
C	0.666476	1.563042	4.742402
C	1.823989	1.252891	5.452459

C	0.067279	2.600881	6.872445
C	0.666476	1.563042	7.582502
C	2.861845	1.852097	4.742402
C	3.171971	3.009665	5.452459
C	1.823989	1.252891	6.872445
C	2.861845	1.852097	7.582502
C	3.171971	3.009665	6.872445
C	2.572774	4.047503	9.002487
C	1.415261	4.357655	9.712417
C	2.572774	4.047503	11.842459
C	0.377405	3.758448	9.002487
C	0.067279	2.600881	9.712417
C	1.415261	4.357655	11.132402
C	0.377405	3.758448	11.842459
C	0.666476	1.563042	9.002487
C	1.823989	1.252891	9.712417
C	0.067279	2.600881	11.132402
C	0.666476	1.563042	11.842459
C	2.861845	1.852097	9.002487
C	3.171971	3.009665	9.712417
C	1.823989	1.252891	11.132402
C	2.861845	1.852097	11.842459
C	3.171971	3.009665	11.132402

FeB_2N_2-(3,0) CNT

C	1.228024	0.000000	0.000000
C	0.614012	1.063500	0.709000
B	0.614012	1.063500	2.127000
Fe	-0.614012	1.063500	3.500000
C	-0.614012	1.063500	0.000000
C	-1.228024	0.000000	0.709000
N	-1.228024	0.000000	2.127000
C	-0.614012	-1.063500	2.836000
C	-0.614012	-1.063500	0.000000
C	0.614012	-1.063500	0.709000
C	0.614012	-1.063500	2.127000
C	1.228024	0.000000	2.836000
C	1.228024	0.000000	4.254000
N	0.614012	1.063500	4.963000
C	0.614012	1.063500	6.381000
C	-0.614012	1.063500	7.090000
B	-1.228024	0.000000	4.963000
C	-1.228024	0.000000	6.381000
C	-0.614012	-1.063500	7.090000
C	-0.614012	-1.063500	4.254000
C	0.614012	-1.063500	4.963000
C	0.614012	-1.063500	6.381000
C	1.228024	0.000000	7.090000
C	1.228024	0.000000	8.508000
C	0.614012	1.063500	9.217000
C	0.614012	1.063500	10.635000
C	-0.614012	1.063500	11.344000
C	-0.614012	1.063500	8.508000
C	-1.228024	0.000000	9.217000
C	-1.228024	0.000000	10.635000
C	-0.614012	-1.063500	11.344000
C	-0.614012	-1.063500	8.508000
C	0.614012	-1.063500	9.217000
C	0.614012	-1.063500	10.635000
C	1.228024	0.000000	11.344000