Supporting Information

Two-dimensional h-BN/C_2N heterostructure as a promising metal-free photocatalyst for overall water-splitting

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Table S1. The optimized structural parameters for h-BN/C_2N (i), h-BN/C_2N (ii), and different strained h-BN/C_2N HSs. All the units are Å.

system	a	b	*c*
h-BN/C_2N (i)	8.572353	8.572353	17.819958
h-BN/C_2N (ii)	8.572399	8.572399	17.818394
ε = -6%	8.058300	8.058300	17.818111
ε = -4%	8.229700	8.229700	17.818111
ε = -2%	8.401200	8.401200	17.818111
ε = 2%	8.744100	8.744100	17.818111
ε = 4%	8.915500	8.915500	17.818111
ε = 6%	9.087000	9.087000	17.818111

Table S2. The calculated bandgaps (E_g), potential difference between water oxidation potential and VBM (ΔV_1), potential difference between CBM and hydrogen potential potential (ΔV_2), and charge transfer from h-BN layer to C_2N layer (ΔQ) in the h-BN/C_2N (i), h-BN/C_2N (ii), and different strained h-BN/C_2N HSs.

system	E_g (eV)	ΔE_1 (V)	ΔE_2 (V)	ΔQ (e)
h-BN/C_2N (i)	2.30	0.70	0.37	0.026
h-BN/C_2N (ii)	2.29	0.69	0.37	0.027
ε = -6%	2.23	0.69	0.31	0.011
ε = -4%	2.29	0.63	0.43	0.016
ε = -2%	2.23	0.53	0.47	0.024
ε = 2%	2.34	0.78	0.33	0.028
ε = 4%	2.42	0.87	0.32	0.030
ε = 6%	2.55	0.91	0.41	0.029

Table S3. The numbers of electrons (Q) carried by N, B, and C atoms in the h-BN/C_2N (i).

	x	y	*x*	Q (*e*)
N	0.000567528	-0.000114659	0.425318423	7.1860
N	0.167206376	0.333256917	0.423130248	7.1873
N	0.333812055	0.666568185	0.422246804	7.1933
N	0.500517398	0.499931672	0.422352068	7.1955
N	0.667148240	0.833231513	0.423108586	7.1894
N	0.833811749	0.166562886	0.423072740	7.1902
N	0.000485359	0.499870203	0.422328280	7.1945
N	0.167174980	0.833198261	0.423418709	7.1880
N	0.333871743	0.166591683	0.423404232	7.1900
N	0.500456481	-0.000099742	0.422541538	7.1975
N	0.667146172	0.333235869	0.422246334	7.1917
N	0.833848410	0.666536929	0.423177606	7.1887
N	0.351778168	-0.002851598	0.611243098	6.1029
N	0.675854270	-0.002857578	0.611129384	6.0869
N	0.675868518	0.659193901	0.611151551	6.0691
N	0.351798772	0.335097244	0.611252989	6.0556
N	0.013814828	0.335087221	0.611132414	6.1069
N	0.013828953	0.659165315	0.611276876	6.0825
B	0.000512153	0.333032580	0.422870968	0.8068
B	0.166971618	0.166298201	0.424754101	0.8008
B	0.333644843	0.499633620	0.422218916	0.8128
B	0.500742735	0.833341051	0.422280629	0.8079
B	0.667387410	0.666770581	0.422923058	0.8035
B	0.834152695	-0.000111137	0.424590012	0.8061
B	0.000562687	0.833476339	0.424784068	0.8039
B	0.167042656	0.666756189	0.422339727	0.8068
B	0.333614282	-0.000105517	0.423256726	0.8068
B	0.500193752	0.333053471	0.422341416	0.8081
B	0.667302403	0.166467331	0.422264321	0.8066
B	0.833916931	0.500180555	0.422233261	0.8113
C	0.349919754	0.838495956	0.611318114	3.4411
C	0.519068900	0.838480862	0.611241339	3.4591
C	0.172472600	0.661040898	0.611314484	3.4727
C	0.172458848	0.491869287	0.611275504	3.4462
C	0.519064371	0.661040359	0.611256978	3.4598
C	0.349911494	0.491884751	0.611278683	3.479
C	0.508580489	0.155804108	0.611313289	3.4293
C	0.677728292	0.155796447	0.611236316	3.4896
C	0.855171931	0.502390878	0.611291329	3.4582
C	0.855161703	0.333228566	0.611249927	3.4424
C	0.508579851	0.333242440	0.611307177	3.4854
C	0.677737602	0.502407964	0.611287779	3.4596

Table S4. The numbers of electrons (Q) carried by N, B, and C atoms in the h-BN/C_2N (ii).

	x	y	*x*	Q (*e*)
N	0.999524112	0.166671133	0.420707349	7.1845
N	0.166245970	0.499983243	0.419823678	7.1924
N	0.332838753	0.833305397	0.420025197	7.1872
N	0.499577732	0.666722991	0.419864393	7.1936
N	0.666170343	0.000005525	0.419732458	7.1881
N	0.832860884	0.333286621	0.419831593	7.1894
N	0.999546190	0.666622500	0.420018416	7.1881
N	0.166183644	0.000006763	0.421186061	7.1866
N	0.332928717	0.333386203	0.419964722	7.1849
N	0.499536900	0.166703248	0.420025905	7.1901
N	0.666266689	0.500024147	0.419860361	7.1935
N	0.832857003	0.833340862	0.420786731	7.1829
N	0.353042306	0.997000120	0.614301280	6.0955
N	0.677112144	0.997021590	0.614178969	6.0862
N	0.677115445	0.659025875	0.614240698	6.0914
N	0.353057796	0.334966394	0.614188297	6.0876
N	0.015148840	0.334931861	0.614228592	6.0672
N	0.015124089	0.659023782	0.614192594	6.0810
B	0.999581725	0.500150789	0.419594533	0.8196
B	0.166019204	0.332995822	0.420333020	0.8059
B	0.332882206	0.666690220	0.419475711	0.8069
B	0.499621923	0.000005272	0.419653279	0.8206
B	0.666583625	0.833494267	0.420224924	0.8059
B	0.833095522	0.166524159	0.420171271	0.8053
B	0.999531122	0.000006626	0.421723999	0.8094
B	0.166046339	0.833555813	0.420710343	0.8048
B	0.332496397	0.166456909	0.420677673	0.8032
B	0.499450072	0.499874147	0.419601440	0.8200
B	0.666202818	0.333332067	0.419477780	0.8086
B	0.833032521	0.667023169	0.420421661	0.8021
C	0.351202222	0.838354611	0.614299159	3.4596
C	0.520350942	0.838349539	0.614291480	3.4359
C	0.173780878	0.660916930	0.614309868	3.4535
C	0.173766256	0.491741127	0.614270249	3.4720
C	0.520332610	0.660897099	0.614262573	3.4743
C	0.351169173	0.491749495	0.614288601	3.4613
C	0.509827644	0.155635444	0.614293138	3.4899
C	0.679030324	0.155682029	0.614282611	3.4423
C	0.856447019	0.502241869	0.614287246	3.4430
C	0.856491758	0.333085909	0.614252077	3.4894
C	0.509837230	0.333076808	0.614306473	3.4325
C	0.6789729120	0.502231624	0.614273597	3.4642

Table S5 Free energy changes (ΔG_H) in HER process of h-BN/C_2N HSs with different hydrogen coverage at different potential. All the unites are eV.

	θ = 0.17	θ = 0.33	θ = 0.50	θ = 0.67	θ = 0.83	θ = 1
U = 0 eV	-1.02	-0.94	-0.11	-0.18	0.26	0.001
U = 0.37 eV	-1.39	-1.31	-0.48	-0.55	-0.11	-0.37

Table S6 The free energy changes for all the reaction steps in OER process of h-BN/C2N HS at different potentials.

	ΔG_1 (eV)	ΔG_2 (eV)	ΔG_3 (eV)	ΔG_4 (eV)
U = 0 eV	1.926	1.24	1.16	0.60
U = 1.23 eV	0.696	0.01	-0.07	-0.63
U = 1.93 eV	-0.004	-0.69	-0.78	-1.33

Table S7. Values used for the entropy and zero-point energy (ZPE) corrections in determining the free energy of reactants, products, and intermediate species adsorbed on catalysts.

system	T×S (eV)	ZPE (eV)
*H	0	0.33
*2H	0.01	0.65
*3H	0.03	0.96
*4H	0.07	1.26
*5H	0.04	1.61
*6H	0.04	1.94
H_2O (0.035bar)	0.68	0.38
H_2	0.40	0.28
*O	0.04	0.26
*OH	0.13	0.52
*OOH	0.20	0.39

Table S8. The fractional coordinates of N, B, and C atoms in the h-BN/C_2N (i).

	x	y	*x*
N	0.000567528	-0.000114659	0.425318423
N	0.167206376	0.333256917	0.423130248
N	0.333812055	0.666568185	0.422246804
N	0.500517398	0.499931672	0.422352068
N	0.667148240	0.833231513	0.423108586
N	0.833811749	0.166562886	0.423072740
N	0.000485359	0.499870203	0.422328280
N	0.167174980	0.833198261	0.423418709
N	0.333871743	0.166591683	0.423404232
N	0.500456481	-0.000099742	0.422541538
N	0.667146172	0.333235869	0.422246334
N	0.833848410	0.666536929	0.423177606
N	0.351778168	-0.002851598	0.611243098
N	0.675854270	-0.002857578	0.611129384
N	0.675868518	0.659193901	0.611151551
N	0.351798772	0.335097244	0.611252989
N	0.013814828	0.335087221	0.611132414
N	0.013828953	0.659165315	0.611276876
B	0.000512153	0.333032580	0.422870968
B	0.166971618	0.166298201	0.424754101
B	0.333644843	0.499633620	0.422218916
B	0.500742735	0.833341051	0.422280629
B	0.667387410	0.666770581	0.422923058
B	0.834152695	-0.000111137	0.424590012
B	0.000562687	0.833476339	0.424784068
B	0.167042656	0.666756189	0.422339727
B	0.333614282	-0.000105517	0.423256726
B	0.500193752	0.333053471	0.422341416
B	0.667302403	0.166467331	0.422264321
B	0.833916931	0.500180555	0.422233261
C	0.349919754	0.838495956	0.611318114
C	0.519068900	0.838480862	0.611241339
C	0.172472600	0.661040898	0.611314484
C	0.172458848	0.491869287	0.611275504
C	0.519064371	0.661040359	0.611256978
C	0.349911494	0.491884751	0.611278683
C	0.508580489	0.155804108	0.611313289
C	0.677728292	0.155796447	0.611236316
C	0.855171931	0.502390878	0.611291329
C	0.855161703	0.333228566	0.611249927
C	0.508579851	0.333242440	0.611307177
C	0.677737602	0.502407964	0.611287779

Table S9. The fractional coordinates of N, B, and C atoms in the h-BN/C_2N (ii).

	x	y	*x*
N	0.999524112	0.166671133	0.420707349
N	0.166245970	0.499983243	0.419823678
N	0.332838753	0.833305397	0.420025197
N	0.499577732	0.666722991	0.419864393
N	0.666170343	0.000005525	0.419732458
N	0.832860884	0.333286621	0.419831593
N	0.999546190	0.666622500	0.420018416
N	0.166183644	0.000006763	0.421186061
N	0.332928717	0.333386203	0.419964722
N	0.499536900	0.166703248	0.420025905
N	0.666266689	0.500024147	0.419860361
N	0.832857003	0.833340862	0.420786731
N	0.353042306	0.997000120	0.614301280
N	0.677112144	0.997021590	0.614178969
N	0.677115445	0.659025875	0.614240698
N	0.353057796	0.334966394	0.614188297
N	0.015148840	0.334931861	0.614228592
N	0.015124089	0.659023782	0.614192594
B	0.999581725	0.500150789	0.419594533
B	0.166019204	0.332995822	0.420333020
B	0.332882206	0.666690220	0.419475711
B	0.499621923	0.000005272	0.419653279
B	0.666583625	0.833494267	0.420224924
B	0.833095522	0.166524159	0.420171271
B	0.999531122	0.000006626	0.421723999
B	0.166046339	0.833555813	0.420710343
B	0.332496397	0.166456909	0.420677673
B	0.499450072	0.499874147	0.419601440
B	0.666202818	0.333332067	0.419477780
B	0.833032521	0.667023169	0.420421661
C	0.351202222	0.838354611	0.614299159
C	0.520350942	0.838349539	0.614291480
C	0.173780878	0.660916930	0.614309868
C	0.173766256	0.491741127	0.614270249
C	0.520332610	0.660897099	0.614262573
C	0.351169173	0.491749495	0.614288601
C	0.509827644	0.155635444	0.614293138
C	0.679030324	0.155682029	0.614282611
C	0.856447019	0.502241869	0.614287246
C	0.856491758	0.333085909	0.614252077
C	0.509837230	0.333076808	0.614306473
C	0.6789729120	0.502231624	0.614273597

Table S10. The fractional coordinates of N, B, and C atoms in the -6% strained h-BN/C_2N HS .

	x	y	*x*
N	0.003921068	-0.000797208	0.474161566
N	0.176243118	0.344122201	0.438019309
N	0.333977000	0.666521545	0.378412279
N	0.503343971	0.501937812	0.391541800
N	0.658133499	0.828387764	0.437832155
N	0.829201238	0.170494675	0.437823437
N	0.001155229	0.497573241	0.391568363
N	0.173916755	0.825765372	0.438389104
N	0.347588633	0.173128909	0.438364469
N	0.498675516	0.999737415	0.391670238
N	0.667292448	0.333137911	0.378410089
N	0.831543276	0.654742314	0.438055053
N	0.334537235	0.997596194	0.616287662
N	0.688713387	0.997592564	0.614074181
N	0.688886676	0.674791893	0.615304311
N	0.334611701	0.320490502	0.615320629
N	0.011695078	0.320380091	0.615370301
N	0.011704958	0.674705077	0.615300226
B	0.002213724	0.337464456	0.422901477
B	0.176943988	0.172961833	0.457024267
B	0.330048133	0.496933850	0.400323702
B	0.504161822	0.831125626	0.400299309
B	0.664290899	0.661617566	0.422913399
B	0.829875598	0.999318449	0.456745971
B	0.003298145	0.825652789	0.457055285
B	0.170068351	0.671108786	0.400503431
B	0.340129990	0.999539298	0.423336755
B	0.498653063	0.328276383	0.400484095
B	0.672725678	0.168245199	0.400293149
B	0.832792185	0.502445478	0.400342802
C	0.345730414	0.839735477	0.616004007
C	0.519752571	0.839670506	0.615152037
C	0.169639481	0.663574926	0.615872905
C	0.169583876	0.489439034	0.615755699
C	0.519842155	0.663597819	0.615404580
C	0.345738869	0.489512998	0.615629549
C	0.503581107	0.155456986	0.616011051
C	0.677657340	0.155498909	0.615162809
C	0.853792699	0.505669915	0.615609106
C	0.853832265	0.331577793	0.615426639
C	0.503657865	0.331610909	0.615874517
C	0.677709154	0.505736845	0.615718503

Table S11. The fractional coordinates of N, B, and C atoms in the -4% strained h-BN/C_2N HS .

	x	y	*x*
N	0.003402847	0.999334498	0.467114031
N	0.172044731	0.337388641	0.434714517
N	0.334376779	0.666552232	0.392594308
N	0.502494576	0.500958552	0.401589922
N	0.664433834	0.831314406	0.435068224
N	0.832641878	0.167826903	0.435075126
N	0.001271305	0.498557521	0.401382924
N	0.170552041	0.829658491	0.435145895
N	0.340342066	0.169331648	0.435101313
N	0.500065935	0.999738206	0.401989901
N	0.667593259	0.333071680	0.392587368
N	0.834234394	0.661641727	0.434806683
N	0.340044547	0.997508321	0.612062671
N	0.683719408	0.997526674	0.611763747
N	0.683738151	0.669344513	0.612209068
N	0.340029025	0.325695375	0.611752955
N	0.011906283	0.325670993	0.612248977
N	0.011861837	0.669357541	0.611763403
B	0.001970084	0.334547329	0.423587878
B	0.172449049	0.169037054	0.451226287
B	0.331971130	0.497528476	0.407441602
B	0.503641976	0.832372687	0.40774589
B	0.667096731	0.664691544	0.423712367
B	0.833305932	0.999467161	0.451314070
B	0.002877912	0.829808978	0.451279818
B	0.168807369	0.669243254	0.407548975
B	0.336927680	0.999572642	0.424066399
B	0.499261938	0.33016408	0.407606839
B	0.670945125	0.167059559	0.407739060
B	0.834157176	0.501921678	0.407401585
C	0.346481438	0.839153970	0.612172325
C	0.518970587	0.839112163	0.612122584
C	0.170303275	0.663004949	0.612113549
C	0.170262364	0.490461123	0.612259435
C	0.518982335	0.662955006	0.612237180
C	0.346441093	0.490476413	0.612149604
C	0.504812166	0.155874983	0.612162759
C	0.677348462	0.155920429	0.612138624
C	0.853473463	0.504574692	0.612146570
C	0.853532997	0.332074946	0.612260951
C	0.504798724	0.332030812	0.612102926
C	0.677288258	0.504548314	0.612241906

Table S12. The fractional coordinates of N, B, and C atoms in the -2% strained h-BN/C_2N HS .

	x	y	*x*
N	0.002848133	0.999363910	0.450025562
N	0.169425568	0.333047095	0.428318869
N	0.335045142	0.666336291	0.409836231
N	0.502123817	0.499753650	0.413488991
N	0.668822211	0.832887985	0.428158950
N	0.835421828	0.166007214	0.427814448
N	0.001911130	0.499407651	0.413264670
N	0.169084786	0.832087173	0.430649963
N	0.336408600	0.166779939	0.430519318
N	0.501428612	0.999538174	0.415185593
N	0.668287977	0.332844705	0.409817386
N	0.835828003	0.665786615	0.428748831
N	0.344731714	0.997674046	0.610544923
N	0.678382737	0.997688723	0.609805931
N	0.678396434	0.664527339	0.610046602
N	0.344696621	0.330846381	0.610140584
N	0.011550610	0.330852065	0.609970374
N	0.011541147	0.664520846	0.610185172
B	0.002266919	0.332820225	0.422830180
B	0.169451530	0.166318220	0.439593458
B	0.334360487	0.498564318	0.415731990
B	0.502860788	0.832932211	0.416323533
B	0.668953941	0.666153944	0.423233092
B	0.835988279	0.999425611	0.438439900
B	0.002555420	0.832450880	0.439821646
B	0.168607787	0.667257809	0.416578237
B	0.335562305	0.999462590	0.425632542
B	0.500902815	0.331827758	0.416603902
B	0.669442488	0.166130032	0.416179240
B	0.835330678	0.500539775	0.415812239
C	0.346791142	0.839034058	0.610411160
C	0.517677089	0.839033181	0.610097493
C	0.170204267	0.662471292	0.610313029
C	0.170185233	0.491578454	0.610161944
C	0.517686786	0.662449021	0.610102381
C	0.346769120	0.491564938	0.610140875
C	0.505436635	0.156314278	0.610401976
C	0.676334927	0.156342086	0.610070535
C	0.852901439	0.503816831	0.610174922
C	0.852923466	0.332932823	0.610069922
C	0.505421068	0.332896371	0.610303831
C	0.676310482	0.503803637	0.610199787

Table S13. The fractional coordinates of N, B, and C atoms in the 2% strained h-BN/C_2N HS .

	x	y	*x*
N	0.000629915	0.999868417	0.423765445
N	0.167286329	0.333243218	0.42288692
N	0.333944598	0.666545299	0.422793743
N	0.500583277	0.499852502	0.422593104
N	0.667249982	0.833180564	0.422897934
N	0.833943005	0.166572859	0.422897032
N	0.000605089	0.499904209	0.422587694
N	0.167296020	0.833206353	0.422936665
N	0.333964809	0.166544348	0.422939029
N	0.500626869	0.999877496	0.422607066
N	0.667272838	0.333208570	0.422790565
N	0.833918562	0.666509205	0.422898479
N	0.356298852	0.997155998	0.611401995
N	0.671220116	0.997177243	0.611423852
N	0.671061590	0.654544600	0.611370302
N	0.356142392	0.339650100	0.611465634
N	0.013686692	0.339792545	0.611367404
N	0.013673669	0.654691568	0.611466312
B	0.000622447	0.333048893	0.422854537
B	0.167048917	0.166279490	0.423831424
B	0.333725022	0.499581584	0.422481075
B	0.500888469	0.833310067	0.422486688
B	0.667456821	0.666710450	0.422870356
B	0.834237714	0.999872396	0.423799616
B	0.000642685	0.833459413	0.423838137
B	0.167165884	0.666766935	0.422516188
B	0.333748292	0.999874088	0.422946133
B	0.500277333	0.332992339	0.422515416
B	0.667456418	0.166448906	0.422482998
B	0.834024634	0.500180466	0.422486956
C	0.350952259	0.838819453	0.611474676
C	0.518171015	0.838813621	0.611450694
C	0.172034600	0.660005042	0.611471655
C	0.172026152	0.492781713	0.611460874
C	0.518077928	0.659913423	0.611455359
C	0.350852704	0.492714530	0.611461932
C	0.509286952	0.155509619	0.611472803
C	0.676518546	0.155526055	0.611450722
C	0.855317649	0.501635063	0.611462605
C	0.855334742	0.334429582	0.611456507
C	0.509180719	0.334328449	0.611465090
C	0.676407651	0.501553434	0.611458583

Table S14. The fractional coordinates of N, B, and C atoms in the 4% strained h-BN/C_2N HS .

	x	y	*x*
N	0.000598326	0.999875718	0.423352588
N	0.167267662	0.333271691	0.422845725
N	0.333927471	0.666546590	0.422845691
N	0.500539309	0.499826177	0.422658552
N	0.667205601	0.833158855	0.422857188
N	0.833922931	0.166597814	0.422857556
N	0.000591102	0.499928920	0.422656577
N	0.167297155	0.833206454	0.422861597
N	0.333966087	0.166545721	0.422863952
N	0.500638201	0.999877161	0.422656835
N	0.667256680	0.333206760	0.422844222
N	0.833875439	0.666483981	0.422848684
N	0.360575921	0.997158602	0.611457486
N	0.666954133	0.997173303	0.611472827
N	0.666841756	0.650302346	0.611424499
N	0.360471635	0.343937721	0.611522776
N	0.013706500	0.344038609	0.611420215
N	0.013699618	0.650400168	0.611533375
B	0.000603787	0.333057618	0.422851333
B	0.167000191	0.166258785	0.423579064
B	0.333692565	0.499554496	0.422547085
B	0.500901169	0.833322735	0.422546258
B	0.667431675	0.666702363	0.422861066
B	0.834236182	0.999872518	0.423566556
B	0.000613943	0.833483571	0.423582554
B	0.167133070	0.666786783	0.422568471
B	0.333730312	0.999874452	0.422906025
B	0.500227301	0.332974244	0.422567598
B	0.667454951	0.166438181	0.422543654
B	0.834018216	0.500211353	0.422551350
C	0.352454250	0.839615236	0.611522453
C	0.517485060	0.839602390	0.611491925
C	0.171264689	0.658500302	0.611518379
C	0.171252527	0.493456091	0.611506055
C	0.517417622	0.658430592	0.611502841
C	0.352383061	0.493415594	0.611507959
C	0.510001460	0.154716162	0.611521484
C	0.675042325	0.154731384	0.611491579
C	0.856140475	0.500929805	0.611512795
C	0.856147432	0.335908804	0.611502327
C	0.509925508	0.335833019	0.611512638
C	0.674966858	0.500877046	0.611508420

Table S15. The fractional coordinates of N, B, and C atoms in 6% strained the h-BN/C_2N HS .

	x	y	*x*
N	0.001045898	0.999801931	0.422044927
N	0.167711890	0.333196134	0.421705108
N	0.334377000	0.666472202	0.421761623
N	0.500986497	0.499748204	0.421607221
N	0.667655935	0.833080998	0.421719954
N	0.834376629	0.166526662	0.421718748
N	0.001040288	0.499857093	0.421603671
N	0.167752043	0.833136751	0.421721691
N	0.334417493	0.166468636	0.421724412
N	0.501094840	0.999802534	0.421620312
N	0.667708886	0.333134064	0.421760854
N	0.834320536	0.666412825	0.421706533
N	0.364075521	0.997270582	0.612935660
N	0.662235590	0.997265422	0.612991810
N	0.662149614	0.646309425	0.612944483
N	0.363985779	0.348153806	0.613015416
N	0.013101145	0.348217812	0.612948231
N	0.013109831	0.646380035	0.613020468
B	0.001051550	0.332990568	0.421733218
B	0.167452819	0.166194489	0.422291563
B	0.334139267	0.499475397	0.421491754
B	0.501357495	0.833246179	0.421499779
B	0.667871764	0.666620055	0.421741960
B	0.834671296	0.999800104	0.422285878
B	0.001058373	0.833403737	0.422293671
B	0.167587678	0.666715124	0.421509175
B	0.334191492	0.999799726	0.421783114
B	0.500678696	0.332896802	0.421509928
B	0.667913244	0.166365264	0.421497124
B	0.834469685	0.50014046	0.421494348
C	0.353780032	0.841081934	0.613003380
C	0.516309279	0.841078306	0.612993944
C	0.169292166	0.656647622	0.613003639
C	0.169289195	0.494112489	0.613011745
C	0.516249400	0.656603419	0.613011769
C	0.353722227	0.494079936	0.613009681
C	0.509961418	0.153449239	0.613004851
C	0.672499906	0.153465502	0.612995494
C	0.856909117	0.500449775	0.613009756
C	0.856919867	0.337929935	0.613013469
C	0.509909534	0.337884401	0.613000188
C	0.672439227	0.500424535	0.613009663

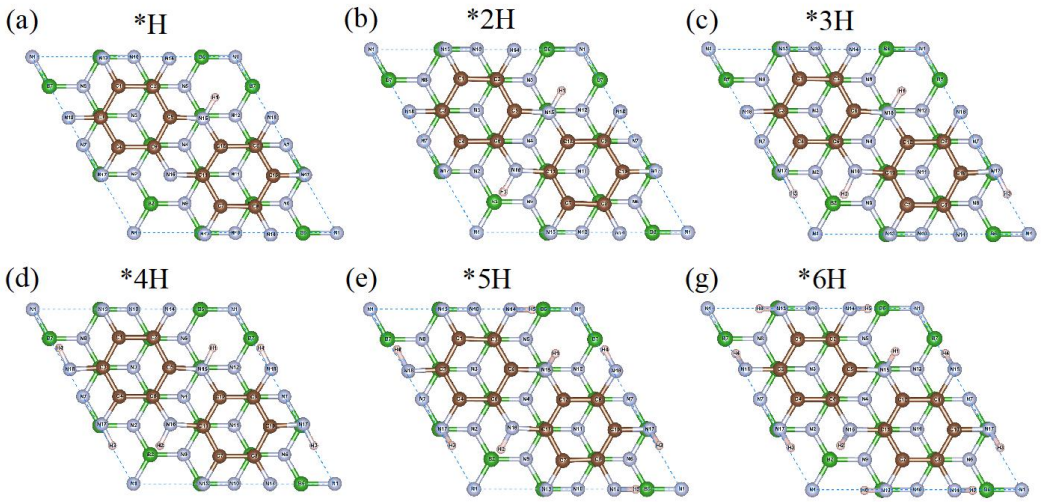

Fig. S1 Top views of optimized geometries of (a) *H, (b) *2H, (c) *3H, (d) *4H, (e) *5H, and (f) *6H intermediates.

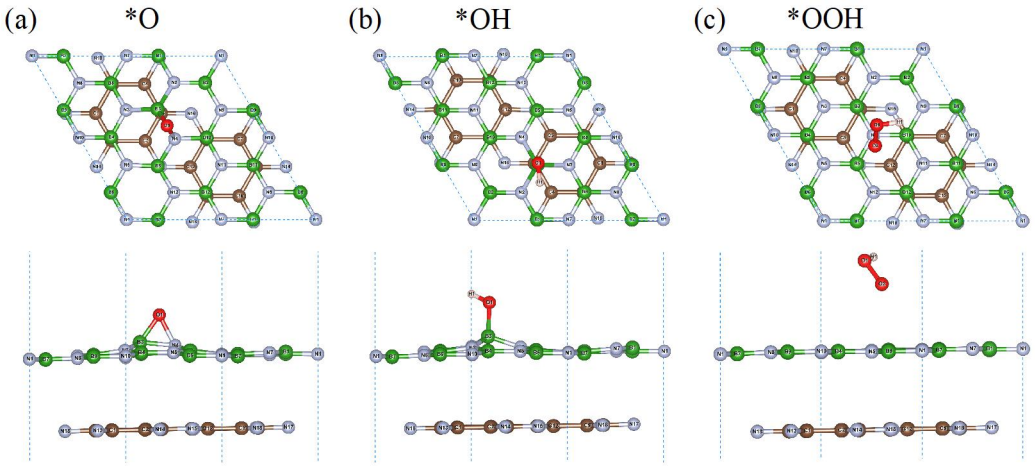

Fig. S2 Top and side views of optimized geometries of (a) *O, (b) *OH, and (c) *OOH intermediates.