

Supporting Information for

C₂N: an excellent catalyst for the hydrogen evolution reaction[†]

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The manuscript was written through contributions of all authors. All authors have given approval to the final version of the manuscript. [†]These authors contribute equally to the work.

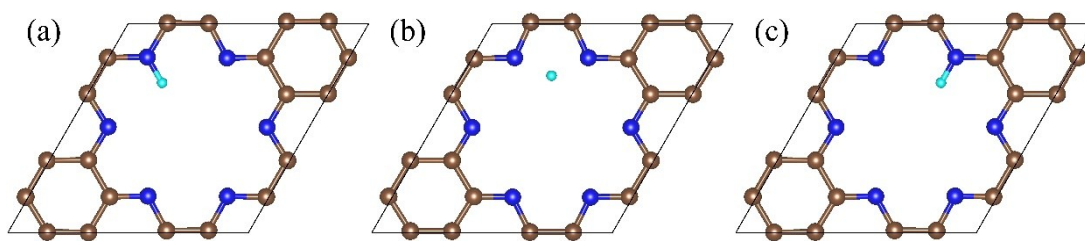


Figure S1: Optimized configures of H atom diffusing from one binding site to an adjacent one. (a) initial state, (b) transitional state and (c) final state. The brown, blue and cyan spheres represent C, N and H atoms, respectively.

Atomic positions:

Initial state

1.0000000000000000		
8.3267563162204059	0.0000000000000000	0.0000000000000000
-4.1633781581102030	7.2112095938051901	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000
N	C	H
6	12	1

Direct

0.8363743094682922	0.5068686710379369	0.5026430932111817
0.5068694451580916	0.8363749229199795	0.5026431179693175
0.5049853872173763	0.1751550636750931	0.5026498169072952
0.1751560037557765	0.5049858168642642	0.5026497981268153
0.8409544048309379	0.8409548139734966	0.5025900478121079
0.1745861396374180	0.1745853822167400	0.5025947048706604
0.0016271295992769	0.6654792430885900	0.5026335226594578
0.6654798253442715	0.0016277381091989	0.5026335221787855
0.1726420012163342	0.6631342119187501	0.5026628677026707
0.0036849283268312	0.8380599877188172	0.5025866949891246
0.3482250476842179	0.8393291259238442	0.5026620026104032
0.8380607158575495	0.0036855689702801	0.5025866819687714
0.1716314175681373	0.0115558307262641	0.5025872972236730
0.3458464032144442	0.0106528462042353	0.5026312033653438
0.6631345073402873	0.1726419420473390	0.5026628587658397

0.0115567956797404	0.1716317617769421	0.5025872771648967
0.8393294166331300	0.3482250232928707	0.5026619732034955
0.0106537865106826	0.3458466541433159	0.5026311719543133
0.7174987642232373	0.7175002901669195	0.5027023498275410

Transitional state

1.0000000000000000

8.3267563162204059	0.0000000000000000	0.0000000000000000
-4.1633781581102030	7.2112095938051901	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

N	C	H
6	12	1

Direct

0.8378384344224119	0.5188294115261153	0.5026294954248809
0.5039068509978889	0.8351951155199863	0.5026316959943150
0.5039060256203536	0.1747380981475748	0.5026318293831503
0.1704043496715663	0.5001840415208105	0.5026316014684812
0.8378381388724683	0.8250364196631231	0.5026299585812403
0.1704044993500357	0.1762466367152233	0.5026316713542596
0.0079396756418504	0.6706370314832429	0.5026329400318508
0.6634257446955020	0.9968746154821309	0.5026310538803028
0.1731112178638159	0.6628249551032811	0.5026334586386956
0.0079396633878211	0.8433299048726731	0.5026332300099233
0.3457639285711009	0.8389536276831644	0.5026334573723372
0.8325050231517173	0.9894478771623401	0.5026304569806024
0.1731111369589939	0.0163126593390697	0.5026337390151998
0.3457640306631262	0.0128362017885557	0.5026334086171967
0.6634257259812082	0.1725785373626372	0.5026312671081480
0.0036571045707515	0.1650011531957800	0.5026311226302171
0.8325049558966580	0.3490845535317897	0.5026303314793876
0.0036570671456344	0.3446827884558223	0.5026310498146752
0.7511928558031000	0.6286111519745556	0.5026282347268388

Final state

1.0000000000000000

8.3267563162204059	0.0000000000000000	0.0000000000000000
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-4.1633781581102030	7.2112095938051901	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000
N	C	H
6	12	1
Direct		
0.8409583934095578	0.5060242586413365	0.5026564715395097
0.5049743648201032	0.8358506596387145	0.5026394917994192
0.5068661739812962	0.1765368053727694	0.5026456171189343
0.1745987909346012	0.5060294846320545	0.5026450491172108
0.8363625147747500	0.8355233010053473	0.5025992243603562
0.1751444699974598	0.1761931483250908	0.5025972013750850
0.0037017401691563	0.6716518248475861	0.5026356624280052
0.6631224037842451	-0.0034806726045685	0.5026315502553519
0.1716441213364302	0.6661023550748235	0.5026438227484904
0.0016214963565802	0.8421701870351885	0.5026087614807592
0.3458428045907915	0.8412195298733678	0.5026420567793821
0.8393232579476814	-0.0028735880029235	0.5026073066294339
0.1726331282289113	0.0155280091331270	0.5026079967628736
0.3482264847027765	0.0149309488447435	0.5026326416974681
0.6654770403338184	0.1698822825131354	0.5026465584622380
0.0106439565892236	0.1708372263205730	0.5026067686778182
0.8380681400370994	0.3403931205807070	0.5026488349531748
0.0115689025140050	0.3459502567520271	0.5026330412996327
0.7175182447575311	0.5060454666248686	0.5026719450265514

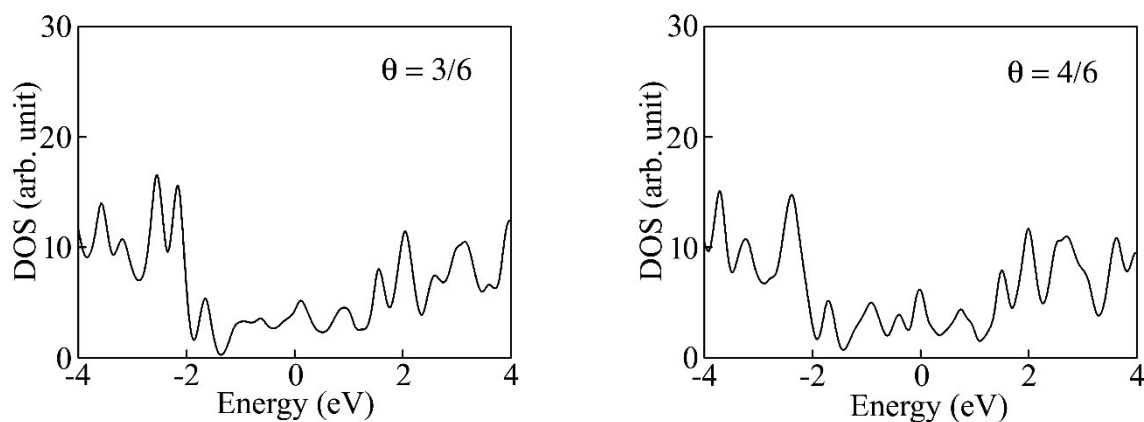


Figure S2: Density of states for C₂N@G at H₋ coverage of 3/6 and 4/6. The Fermi level is set at 0 eV.