Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

N_2 Activation on Al Metal Clusters: Catalyzing role of BN-doped Graphene Support

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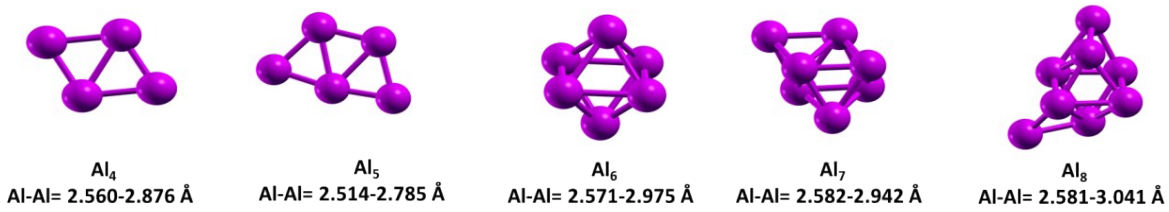

Figure S1: Optimized structures of ground state Al_{4-8} clusters

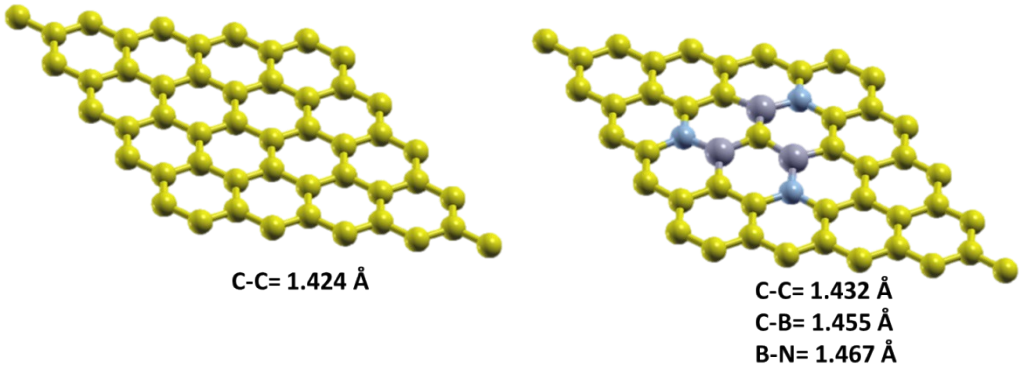

Figure S2: Optimized structures of Graphene and BN-doped graphene

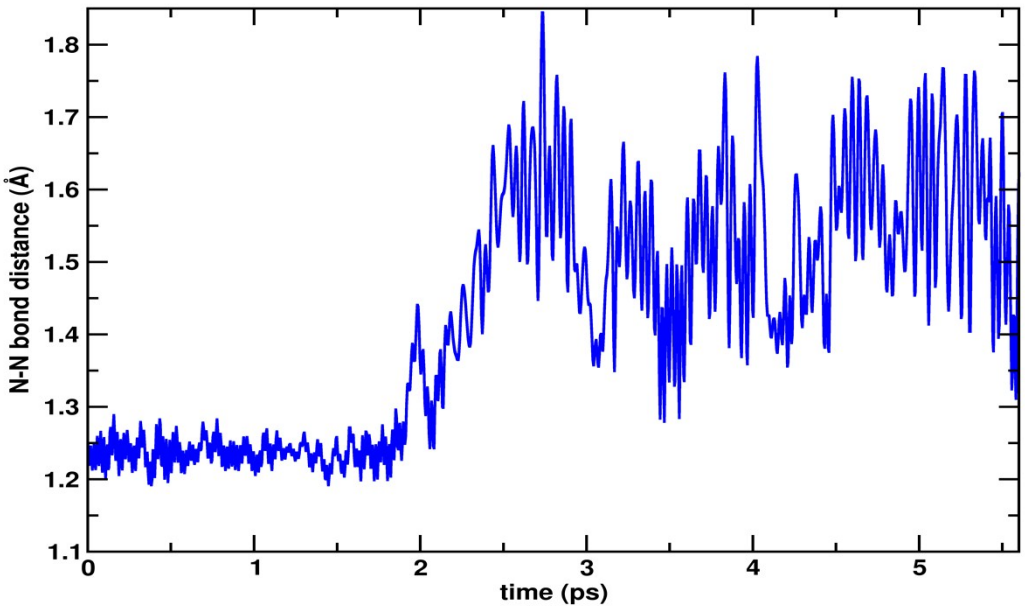

Figure S3: N-N bond length fluctuations in Al_4@BN_graphene-N_2 complex at 300 K.

Table S1 N_2 activation on Li_4/Ru_4 clusters with vibrational frequencies

System	Li-N/Ru-N(Å)	C-Li/C-Ru(Å)	N-N(Å)	Vib. Frequency(cm^{-1})
N_2@Li_4	2.221-2.244		1.125	2246
N_2@Li_4_BN	2.104-2.134	2.051	1.146	2130
N_2@Ru_4	1.961-1.966		1.203	1548
N_2@Ru_4_BN	1.947-1.948	2.093	1.221	1541

Table S2 Bader charges for Al_n@graphene and Al_n@BN_graphene (n=4-8)

S.No.	q(Al_n)	q(graphene)	q(Al_n)	q(BN_graphene)
n=4	0.27	-0.27	0.52	-0.52
n=5	0.04	-0.04	0.64	-0.64
n=6	0.06	-0.06	0.66	-0.66
n=7	0.57	-0.57	0.76	-0.76
n=8	0.03	-0.03	0.42	-0.42

2. Cartesian coordinates of optimized structures given in Figure 1, 2, 3 (in Å)

(i) Cartesian Coordinates for Optimized structures given in Figure 1(in Å)

$N_2@Al_4$

6

Al	5.105913	10.965635	7.267518
Al	6.522225	11.605378	9.299214
Al	4.493008	10.199669	9.812287
Al	3.072368	9.585839	7.755453
N	3.901717	9.571952	11.730426
N	3.036352	9.107137	11.103495

$N_2@Al_5$

7

Al	5.677597	11.050996	6.814899
Al	3.475993	9.305943	7.895963
Al	4.944396	11.047635	9.413311
Al	7.261175	11.972760	8.631177
Al	7.390785	12.986024	6.208226
N	3.989480	10.651749	6.165250
N	2.912642	10.131430	6.036777

$N_2@Al_6$

8

Al	6.066570	9.721775	7.401635
Al	6.560998	8.957557	10.239793
Al	8.154300	8.488975	8.269573
Al	8.109553	11.282422	7.509412
Al	8.586171	10.543437	10.270410
Al	6.530456	11.847710	9.461083
N	3.270471	10.129140	8.906644
N	3.432254	9.923135	9.993792

$N_2@Al_7$

9

Al	6.114725	9.919903	7.324778
Al	6.152464	8.293381	9.723842
Al	5.046188	9.336045	12.017154
Al	7.400722	10.212898	11.205797

Al	8.453749	9.459878	8.971171
Al	7.250492	11.865511	8.810153
Al	5.054041	10.747004	9.688832
N	5.582141	8.047130	6.735938
N	5.708496	7.982383	7.948075

$N_2@Al_8$

10

N	3.914707	8.419539	7.758504
N	4.161070	8.897655	6.716479
Al	6.190067	9.667361	7.322135
Al	7.450591	8.354021	9.183712
Al	6.344023	10.791967	9.973943
Al	4.803048	8.700170	9.663148
Al	6.427484	7.455451	11.533750
Al	8.085210	9.484446	11.404249
Al	6.708897	11.349345	12.715311
Al	4.946287	9.549468	12.030749

$Al_4@graphene$

54

C	7.824435	8.607874	4.897331
C	7.105290	7.366684	4.895521
C	7.820906	6.131702	4.856634
C	9.251861	6.133111	4.831927
C	9.966280	7.370540	4.827726
C	9.251030	8.608531	4.852552
C	7.107181	4.892568	4.841951
C	5.678325	4.892280	4.841470
C	4.961892	6.128601	4.868705
C	5.678042	7.360454	4.918662
C	3.530504	6.131018	4.859940
C	2.817349	4.894645	4.836079
C	3.533091	3.656459	4.827757
C	4.962150	3.655976	4.828920
C	2.814277	7.369879	4.847704
C	1.386107	7.370157	4.815620
C	0.673407	6.131699	4.814494
C	1.387241	4.893673	4.820957
C	0.673721	8.608768	4.809103
C	1.387124	9.846509	4.815680
C	2.813026	9.845005	4.854529
C	3.521732	8.606628	4.888316

C	0.674089	11.086634	4.810073
C	1.386766	12.323657	4.816359
C	2.815752	12.324769	4.841258
C	3.527395	11.088119	4.875885
C	2.817356	2.419438	4.825416
C	1.387913	2.418152	4.817877
C	0.673565	3.655916	4.822490
C	4.954131	11.097137	4.927573
C	5.675636	12.327752	4.876066
C	7.106420	12.323246	4.860446
C	7.821694	13.559537	4.825203
C	7.107297	14.798716	4.822028
C	5.677592	14.799969	4.826583
C	4.960581	13.563666	4.844462
C	9.252755	13.561132	4.812556
C	9.966744	14.799114	4.803564
C	9.252804	16.037690	4.809208
C	7.822961	16.035644	4.818588
C	7.825032	11.085958	4.878697
C	9.253013	11.084616	4.842695
C	9.966533	12.322673	4.816059
C	9.967074	17.276050	4.811332
C	9.966562	9.846758	4.838499
C	7.118824	9.847993	4.938794
C	5.678062	9.851790	5.009250
C	3.531702	13.562931	4.837916
C	0.673573	1.181084	4.815754
C	4.954601	8.599398	4.983872
Al	5.437393	9.586346	7.396873
Al	4.060337	7.746288	8.589570
Al	5.125251	9.407803	10.160543
Al	6.487996	11.237446	9.036545

Al_5@graphene

55

C	9.876211	12.428890	4.991746
C	9.163669	13.661915	4.991221
C	7.740729	13.661897	4.991791
C	7.027778	12.428614	4.989012
C	7.740476	11.195243	4.989492
C	9.163518	11.195644	4.990265
C	5.604494	12.429503	4.987264
C	4.891717	13.662057	4.989288
C	5.604907	14.894906	4.991808
C	7.027893	14.894779	4.991155
C	9.876408	14.895320	4.992265
C	9.163696	16.128188	4.991343
C	7.740711	16.127986	4.992164
C	4.890830	11.196105	4.984038
C	5.604478	9.961610	4.987707
C	3.468833	13.661698	4.990964
C	2.756146	12.428448	4.987185
C	1.333496	12.429232	4.991256

C	0.620791	11.196025	4.991058
C	1.333380	9.963066	4.991186
C	2.756052	9.962513	4.986849
C	3.467826	11.195637	4.983889
C	0.620684	8.729768	4.991172
C	1.333040	7.496625	4.991624
C	2.755998	7.496104	4.990477
C	3.468388	8.729101	4.990160
C	3.469142	6.263360	4.991794
C	2.756508	5.030298	4.991212
C	1.333511	5.030815	4.991908
C	0.620481	6.263462	4.990663
C	3.469307	3.797339	4.992207
C	2.756491	2.564196	4.991340
C	1.333536	2.564757	4.992147
C	0.620797	3.797588	4.991226
C	4.892238	3.797218	4.991291
C	5.605013	5.030234	4.991989
C	4.892054	6.262919	4.990608
C	5.604868	7.495732	4.991006
C	7.027923	7.496036	4.990406
C	7.740777	6.263364	4.992011
C	7.027954	5.030254	4.991207
C	7.741104	8.728932	4.990597
C	9.163900	8.729677	4.991000
C	9.876603	7.496976	4.992302
C	9.163765	6.263714	4.991307
C	4.891315	8.728125	4.988588
C	7.028330	9.961764	4.987283
C	9.876441	9.963053	4.991847
C	0.620874	1.331515	4.991350
C	9.876489	17.361530	4.992256
Al	5.399451	10.732038	8.351211
Al	3.302172	11.188214	9.635516
Al	3.426557	10.340443	12.088614
Al	5.698447	10.732854	11.094304
Al	7.119215	9.252308	9.645871

Al_6@graphene

56

C	7.832950	8.626739	4.833382
C	7.119980	7.392547	4.849483
C	7.832681	6.160968	4.885093
C	9.256689	6.161204	4.895218
C	9.969065	7.394354	4.886886
C	9.258016	8.627790	4.859290
C	5.696788	7.393160	4.834559
C	4.985599	6.160658	4.873999
C	5.697483	4.928015	4.890771
C	7.121115	4.927994	4.892199
C	3.561726	6.160927	4.885011
C	2.849448	4.927970	4.896282
C	3.561457	3.695099	4.894082

C	4.985197	3.695349	4.890978
C	2.849902	7.393693	4.873562
C	1.426043	7.394184	4.888559
C	0.713940	6.161473	4.887824
C	1.425690	4.928210	4.892075
C	0.714029	8.627032	4.890706
C	1.425508	9.860108	4.877866
C	2.848550	9.860617	4.835272
C	3.560705	8.626926	4.831893
C	3.560446	11.094348	4.800923
C	2.849459	12.326890	4.844489
C	1.426137	12.326165	4.880548
C	0.713949	11.093319	4.890220
C	2.849255	2.462348	4.887912
C	1.425546	2.462169	4.891802
C	0.713513	3.695472	4.886301
C	3.560762	13.560496	4.856115
C	4.984196	13.561385	4.829891
C	5.696573	14.793661	4.867168
C	7.120293	14.793976	4.867192
C	7.832237	13.561537	4.836278
C	7.119196	12.329981	4.780237
C	5.695105	12.329750	4.768149
C	9.256196	13.560731	4.867577
C	9.968932	12.327778	4.864386
C	9.258033	11.095157	4.833544
C	7.833214	11.095636	4.786324
C	7.832974	16.025900	4.891646
C	9.256675	16.025794	4.897589
C	9.968706	14.792854	4.891848
C	7.121040	9.860663	4.782503
C	4.984429	8.625425	4.795383
C	5.695645	9.860889	4.761774
C	4.983425	11.096369	4.754914
C	9.968889	9.861690	4.857624
C	9.968694	17.258926	4.903259
C	0.714205	1.228754	4.890977
Al	7.654287	11.522788	8.144271
Al	7.976581	8.608303	8.305222
Al	6.202975	8.516258	10.168515
Al	8.600413	10.267588	10.178572
Al	5.894085	11.449791	10.011360
Al	5.295664	9.801157	8.128017

Al_7@graphene

57

C	7.833261	8.623047	4.925725
C	7.116683	7.388729	4.922889
C	7.826537	6.160422	4.913527
C	9.251582	6.161645	4.911709
C	9.963360	7.392595	4.911008

C	9.253688	8.626401	4.913318
C	5.689927	7.382502	4.936437
C	4.976797	6.156070	4.921311
C	5.691344	4.925690	4.912636
C	7.113353	4.927000	4.912339
C	3.552811	6.159128	4.918846
C	2.842018	4.928151	4.913217
C	3.554616	3.695497	4.912081
C	4.977635	3.695052	4.911197
C	2.838501	7.390933	4.921946
C	1.415734	7.394328	4.912829
C	0.706370	6.161011	4.911176
C	1.418051	4.929041	4.912140
C	0.705942	8.626729	4.912686
C	1.418110	9.860918	4.914513
C	2.837524	9.860550	4.927154
C	3.543775	8.622169	4.939814
C	3.548050	11.098435	4.929614
C	2.840413	12.330067	4.914152
C	1.416884	12.327344	4.911161
C	0.706417	11.095484	4.911824
C	2.842139	2.463296	4.911965
C	1.418673	2.462505	4.911994
C	0.707330	3.695720	4.912042
C	3.553543	13.561809	4.913044
C	4.976801	13.563496	4.913709
C	5.690784	14.794655	4.910918
C	7.112978	14.793902	4.911998
C	7.825513	13.559799	4.913200
C	7.115243	12.329863	4.920873
C	5.688698	12.333989	4.927564
C	9.250433	13.559686	4.911784
C	9.962071	12.328145	4.910778
C	9.253155	11.093911	4.913350
C	7.831999	11.096955	4.926136
C	7.825914	16.025848	4.911927
C	9.249675	16.026161	4.912201
C	9.961183	14.793132	4.911897
C	7.129547	9.859900	4.950238
C	5.687316	9.862254	5.000099
C	9.963703	9.860528	4.912906
C	9.961748	17.259168	4.911753
C	4.968277	11.108909	4.953464
C	0.707397	1.229949	4.911121
C	4.967476	8.610063	4.968395
Al	5.712510	9.629645	7.181464
Al	4.096487	9.185866	9.186377
Al	4.923550	10.544041	11.231577
Al	6.388982	11.158565	9.186646
Al	7.473123	9.676953	11.008793
Al	5.409640	7.892153	11.009108
Al	6.959262	8.179376	8.962631

Al_8@graphene

58

C	7.796332	8.653712	4.742520
C	7.083665	7.420452	4.745070
C	7.795034	6.187535	4.747184
C	9.218536	6.187549	4.748195
C	9.930622	7.420792	4.748470
C	9.219167	8.653691	4.746343
C	5.659788	7.419580	4.744867
C	4.947023	6.186936	4.746956
C	5.659096	4.954478	4.747719
C	7.082801	4.954539	4.747924
C	3.523371	6.187654	4.748404
C	2.811294	4.954488	4.749100
C	3.523330	3.721681	4.748880
C	4.947068	3.721409	4.748296
C	2.810993	7.420355	4.747445
C	1.387477	7.420802	4.748575
C	0.675539	6.187591	4.749060
C	1.387620	4.954773	4.749196
C	0.675627	8.653671	4.748342
C	1.387523	9.886953	4.748495
C	2.811056	9.886694	4.747654
C	3.522117	8.653464	4.746009
C	3.522996	11.120298	4.748058
C	2.811211	12.353071	4.748364
C	1.387592	12.353062	4.748806
C	0.675628	11.119834	4.748505
C	2.811307	2.488369	4.749002
C	1.387620	2.488603	4.749178
C	0.675600	3.721500	4.749221
C	3.523373	13.586181	4.748636
C	4.946993	13.586203	4.748114
C	5.659063	14.819293	4.748492
C	7.082737	14.819029	4.748446
C	7.794848	13.586238	4.748567
C	7.083054	12.353003	4.747401
C	5.659158	12.353631	4.747294
C	9.218514	13.585967	4.748391
C	9.930630	12.353178	4.748640
C	9.218950	11.119971	4.747381
C	7.795791	11.120540	4.745004
C	7.794685	16.052304	4.748777
C	9.218410	16.052042	4.748964
C	9.930543	14.819170	4.748755
C	7.085031	9.886868	4.743436
C	5.659520	9.887908	4.748714
C	9.930715	9.887051	4.748257
C	9.930580	17.285411	4.748824
C	4.946433	11.121365	4.746752
C	0.675551	1.255191	4.749113
C	4.946053	8.652290	4.746780
Al	5.737757	9.246016	7.879353
Al	7.584365	8.480153	9.447030
Al	6.406437	11.016439	9.884274
Al	4.375171	8.985442	10.006195
Al	6.148734	7.799139	11.527486
Al	8.074625	9.869918	11.541963

Al	6.952027	10.351106	13.807265
Al	5.083370	10.366236	12.033360

(ii) Cartesian Coordinates of Optimized structures given in Figure 2 (in Å)

Al_4@BN_graphene

54

C	7.826342	16.040476	4.742189
C	7.114118	14.813054	4.755341
C	7.827804	13.579761	4.770242
C	9.255010	13.561930	4.734768
C	9.962304	14.800721	4.723914
C	9.252499	16.037768	4.732175
C	9.978566	12.331274	4.741432
C	9.257102	11.109542	4.806094
C	7.844951	11.135210	4.913395
C	7.119949	12.357912	4.867594
C	5.682761	14.802466	4.772006
C	4.979948	13.571368	4.827733
C	3.478117	11.080781	4.951022
C	2.795639	12.312413	4.836325
C	3.545677	13.550458	4.814406
C	2.780160	9.837782	4.902305
C	1.369043	9.841515	4.789171
C	0.672335	11.088848	4.764688
C	1.375376	12.328689	4.778086
C	2.800446	7.383317	4.843949
C	1.383167	7.371349	4.763166
C	0.660128	8.606562	4.750816
C	0.682065	6.130694	4.738772
C	1.389490	4.892684	4.760202
C	2.820503	4.906513	4.780854
C	3.539109	6.147695	4.838429
C	3.537157	3.658764	4.771930
C	2.831315	2.416478	4.776249
C	1.394113	2.418456	4.771200
C	0.669336	3.650117	4.767650
C	4.962865	3.651526	4.760977
C	5.684694	4.881398	4.780526
C	4.987069	6.114865	4.861036
C	5.680638	9.853981	5.418602
C	5.711230	7.320588	5.007202
C	7.131455	7.340230	4.934805
C	9.250984	8.591441	4.848878
C	9.953460	9.843369	4.809058
C	7.111882	4.893396	4.772854
C	7.837427	6.120533	4.811116
C	9.263550	6.125134	4.776368
C	9.970475	7.367780	4.789119
C	0.673769	1.188627	4.768323
C	9.968079	17.273715	4.747078

N	5.710401	12.382381	4.924539
N	3.456517	8.605361	4.974671
N	7.861676	8.554112	4.973782
B	4.975281	11.133942	5.132346
B	7.142882	9.819718	5.138580
B	4.905444	8.580623	5.248345
Al	5.478580	9.702635	7.461964
Al	6.489694	11.147195	9.312717
Al	4.989963	9.321417	10.178294
Al	4.049823	7.781600	8.426310

Al_5@BN_graphene

55

C	0.699347	3.705549	4.903265
C	1.418848	4.942740	4.895644
C	2.839858	4.956671	4.896234
C	3.551587	3.715153	4.883586
C	2.849148	2.479352	4.882849
C	1.417389	2.481115	4.884056
C	3.556446	6.196068	4.942143
C	4.997279	6.167277	4.969131
C	5.690491	4.933340	4.907035
C	4.969838	3.705836	4.880440
C	5.718990	7.373177	5.115474
C	7.134207	7.382306	5.084297
C	7.835712	6.168703	4.953733
C	7.111376	4.942809	4.909424
C	9.246654	8.630974	4.986509
C	9.959461	7.411087	4.914824
C	9.257756	6.168920	4.912038
C	0.715327	6.175579	4.894888
C	1.416216	7.409209	4.910523
C	2.827839	7.421715	4.967329
C	2.799903	9.876449	5.023279
C	1.398378	9.872625	4.927601
C	0.688392	8.638904	4.906595
C	3.498353	11.106639	5.030270
C	2.815137	12.337067	4.912304
C	1.400042	12.350474	4.879024
C	0.700128	11.113033	4.891262
C	5.682064	9.887599	5.724950
C	9.946284	9.873923	4.957138
C	9.249122	11.135105	4.981670
C	7.844347	11.159189	5.111886
C	7.126677	12.380089	5.048368
C	7.827373	13.594261	4.938071
C	9.251187	13.575673	4.910955
C	9.971055	12.352001	4.915674
C	7.115472	14.825785	4.896393
C	5.687940	14.812499	4.892098
C	4.988833	13.585742	4.936504
C	9.956809	14.809047	4.890731
C	9.247282	16.042039	4.888318

C	7.825442	16.045470	4.885538
C	3.561179	13.568895	4.909978
C	9.958576	17.273521	4.886490
C	0.698672	1.257533	4.879032
N	7.854893	8.599472	5.139083
N	3.495926	8.643940	5.097055
N	5.713298	12.396346	5.061844
B	7.145278	9.848309	5.363892
B	4.930368	8.636691	5.337590
B	4.983076	11.159452	5.276289
Al	5.245374	10.315551	7.647631
Al	3.891033	11.736568	9.136447
Al	4.215185	11.038778	11.848505
Al	5.605667	9.795564	10.191174
Al	2.484575	12.707656	10.985095

Al_6@BN_graphene

56

C	7.860557	11.134175	5.230365
C	7.123011	12.354205	5.065165
C	7.828042	13.564150	4.885964
C	9.254704	13.545924	4.846867
C	9.976816	12.318033	4.845374
C	9.266813	11.100387	4.970768
C	9.957600	14.775492	4.775051
C	9.252613	16.009151	4.753704
C	7.831423	16.012924	4.745439
C	7.121544	14.787967	4.787409
C	4.995143	13.551303	4.873693
C	5.690425	14.779123	4.791336
C	9.965159	17.239280	4.752035
C	3.567186	13.534830	4.821177
C	2.821459	12.301073	4.830826
C	1.406297	12.316608	4.759885
C	0.708236	11.079267	4.761586
C	1.404619	9.839322	4.799521
C	2.808136	9.839393	4.918568
C	3.505757	11.074025	4.962814
C	2.833486	7.389496	4.819707
C	1.416752	7.381712	4.767818
C	0.696036	8.605600	4.774380
C	0.716330	6.143667	4.766045
C	1.418666	4.912118	4.758971
C	2.842126	4.924977	4.743172
C	3.560388	6.164016	4.785095
C	3.554879	3.685268	4.741490
C	4.976749	3.673084	4.744821
C	5.695601	4.899473	4.754106
C	5.003332	6.134923	4.817346
C	2.855045	2.446290	4.758007
C	1.420456	2.447963	4.757641
C	0.699549	3.672835	4.790658
C	7.116293	4.910267	4.757896

C	7.841776	6.134296	4.820801
C	7.142077	7.348045	4.969659
C	5.722481	7.337874	4.980155
C	9.262782	6.131137	4.791853
C	9.961770	7.376859	4.804449
C	9.249680	8.589733	4.925683
C	0.704158	1.223435	4.753848
C	9.949178	9.840720	4.902816
C	5.666450	9.845167	5.620953
N	5.717681	12.367295	5.022330
N	3.496140	8.610584	4.963744
N	7.865796	8.549952	5.127740
B	4.987826	11.120867	5.226913
B	7.159986	9.796439	5.440926
B	4.935639	8.599869	5.218423
Al	5.549948	9.788866	7.715046
Al	6.052057	11.714972	9.466855
Al	8.567035	10.520968	10.000890
Al	7.865708	8.494506	8.534779
Al	7.981355	11.359953	7.685678
Al	5.843601	9.079130	10.159268

Al_7@BN_graphene

57

C	7.844865	11.145365	4.918152
C	7.122614	12.361667	4.918899
C	7.822519	13.578589	4.884024
C	9.244275	13.559260	4.875546
C	9.968701	12.334068	4.868270
C	9.253697	11.117723	4.869595
C	9.950781	14.790471	4.876116
C	9.241185	16.022809	4.877958
C	7.819399	16.024659	4.872107
C	7.107532	14.807775	4.872452
C	4.979921	13.572916	4.878716
C	5.679284	14.794865	4.864418
C	9.954050	17.253289	4.873497
C	3.554640	13.551421	4.873556
C	2.805453	12.320426	4.874561
C	1.393858	12.332249	4.863739
C	0.695819	11.092954	4.872989
C	1.391310	9.852367	4.882554
C	2.795727	9.854185	4.916649
C	3.487934	11.088038	4.927483
C	2.814631	7.393140	4.877259
C	1.406701	7.388244	4.869350
C	0.681949	8.618619	4.876169
C	0.710683	6.156475	4.867748
C	1.410612	4.922926	4.870137
C	2.830488	4.932379	4.870193
C	3.546514	6.169837	4.871585
C	3.542843	3.693038	4.866501
C	4.961094	3.682560	4.859209

C	5.681939	4.906335	4.857755
C	4.985695	6.134017	4.866625
C	2.841058	2.459093	4.868812
C	1.411651	2.460835	4.866440
C	0.693493	3.686082	4.866150
C	7.104262	4.921311	4.867170
C	7.830818	6.143544	4.874371
C	7.126935	7.358882	4.900344
C	5.712354	7.341782	4.910689
C	9.254120	6.145852	4.868873
C	9.957911	7.389499	4.860426
C	9.249751	8.606072	4.863227
C	0.693676	1.237195	4.861363
C	9.942696	9.852069	4.863981
C	5.681986	9.858217	5.333323
N	5.707535	12.381570	4.931864
N	3.484227	8.618735	4.928207
N	7.853013	8.574709	4.909701
B	4.977408	11.144004	5.066513
B	7.147118	9.827169	5.044554
B	4.921406	8.604644	5.052127
Al	6.960439	8.208503	9.074620
Al	5.449351	7.903006	11.160908
Al	7.526418	9.616048	11.169008
Al	6.488931	11.158901	9.374125
Al	4.995130	10.553689	11.396013
Al	4.188310	9.221854	9.328346
Al	5.767867	9.733256	7.320266

Al_8@BN_graphene

58

C	7.826043	11.171512	4.902169
C	7.103157	12.390436	4.892221
C	7.803616	13.607985	4.796468
C	9.225896	13.590322	4.749202
C	9.948669	12.366882	4.732907
C	9.230972	11.148342	4.778057
C	9.931689	14.823021	4.732997
C	9.221650	16.054575	4.729056
C	7.800023	16.057639	4.732061
C	7.090287	14.836416	4.765582
C	4.965389	13.597557	4.823115
C	5.662948	14.823718	4.761695
C	9.935097	17.284491	4.721229
C	3.536505	13.579254	4.793172
C	2.789878	12.347605	4.816278
C	1.376999	12.360535	4.746620
C	0.676673	11.124164	4.748146
C	1.374958	9.885567	4.788067
C	2.779889	9.885366	4.892023
C	3.474319	11.119876	4.937031
C	2.801447	7.433223	4.795480
C	1.390713	7.423583	4.743639

C	0.666709	8.653690	4.750474
C	0.690454	6.190371	4.713560
C	1.391564	4.956275	4.714025
C	2.812167	4.967372	4.726194
C	3.529880	6.204620	4.765940
C	3.526064	3.725579	4.727935
C	4.944694	3.716771	4.728761
C	5.664666	4.943294	4.730402
C	4.969021	6.174301	4.775682
C	2.824804	2.488269	4.739297
C	1.393298	2.490145	4.718270
C	0.674429	3.716743	4.715615
C	7.084932	4.954178	4.731822
C	7.810657	6.177832	4.750968
C	7.109851	7.395363	4.842797
C	5.693102	7.379384	4.883348
C	9.231164	6.179548	4.724381
C	9.936039	7.421158	4.718860
C	9.222784	8.639908	4.759689
C	0.676117	1.265477	4.714182
C	9.923694	9.885677	4.748959
C	5.669310	9.885719	5.426227
N	5.692547	12.411987	4.947174
N	3.465586	8.654045	4.915576
N	7.834053	8.603703	4.867983
B	4.963213	11.168586	5.139951
B	7.126747	9.855166	5.089899
B	4.907766	8.641473	5.096896
Al	5.079458	10.006419	11.715735
Al	6.047869	7.565992	10.997886
Al	7.906903	9.556415	11.261727
Al	6.968180	10.836181	13.401252
Al	4.436874	8.951229	9.465744
Al	6.398491	10.967933	9.691778
Al	7.475045	8.448576	8.991591
Al	5.825225	9.639409	7.449727

(iii) Cartesian Coordinates for Optimized structure given in Figure 3 (in Å)

N_2@Al_4@BN_graphene

56

C	7.859273	16.101586	4.703601
C	7.145410	14.874911	4.719728
C	7.860240	13.642531	4.745519
C	9.288403	13.623831	4.708656
C	9.997356	14.861238	4.700141
C	9.286063	16.098322	4.700634
C	7.152126	12.421650	4.861670
C	5.012533	13.631842	4.794768
C	5.714422	14.864504	4.725754

C	10.011800	12.393591	4.710992
C	9.286981	11.173854	4.774506
C	7.877454	11.199461	4.898965
C	5.716222	9.916371	5.455819
C	3.577025	13.610268	4.766208
C	2.825776	12.374557	4.800351
C	3.509847	11.143810	4.948227
C	2.812626	9.901863	4.912675
C	1.401769	9.902149	4.780931
C	0.704234	11.147423	4.734238
C	1.406179	12.389129	4.733441
C	2.837064	7.444773	4.843700
C	1.418411	7.434317	4.748923
C	0.693821	8.666995	4.736633
C	3.572199	6.209676	4.818775
C	2.852011	4.966797	4.736295
C	1.421950	4.954416	4.711274
C	0.716094	6.193806	4.708454
C	5.017607	6.177961	4.844609
C	5.715089	4.942266	4.746302
C	4.993927	3.712645	4.711803
C	3.567769	3.720145	4.713428
C	5.742510	7.386131	4.985245
C	7.163900	7.401982	4.914370
C	7.869495	6.180853	4.784168
C	7.141486	4.953219	4.737931
C	9.281966	8.652616	4.810693
C	10.000189	7.428908	4.742339
C	9.294792	6.183934	4.737623
C	0.699756	3.711797	4.713650
C	1.424274	2.479352	4.707187
C	2.862035	2.476253	4.712599
C	9.981791	9.905435	4.765290
C	0.703515	1.248672	4.711990
C	10.000592	17.333598	4.707978
N	5.740884	12.445437	4.924956
N	3.499624	8.668371	4.983938
N	7.889860	8.616874	4.943379
N	3.903494	10.213252	10.409288
N	2.684572	10.062978	10.379000
B	5.004222	11.195419	5.151147
B	7.176556	9.882104	5.125776
B	4.952853	8.658598	5.194347
Al	5.906752	10.047116	7.568451
Al	3.364099	9.987420	8.451303
Al	5.736943	10.467629	10.179768
Al	7.941559	11.037865	8.930180

N_2@Al_5@BN_graphene

57

N	5.623276	12.499335	5.126403
N	7.764362	8.689745	5.239496
N	3.394703	8.739648	5.186518

N	5.556983	9.114163	11.961279
N	6.174269	9.215824	10.876474
C	7.033294	12.476519	5.126826
C	7.735778	13.692210	5.008306
C	7.023226	14.921607	4.962387
C	5.597819	14.912568	4.954839
C	4.896991	13.686364	4.997212
C	9.157515	13.674364	4.982364
C	9.879399	12.449431	4.999541
C	9.161740	11.232554	5.082250
C	7.755342	11.258029	5.208961
C	7.733370	16.143978	4.949828
C	9.154975	16.140730	4.946068
C	9.864111	14.908237	4.953369
C	9.851623	9.970703	5.061594
C	9.154084	8.725158	5.091504
C	9.867443	7.505959	5.000391
C	9.162915	6.266860	4.991010
C	7.742657	6.265991	5.039373
C	7.039185	7.482031	5.179328
C	7.018742	5.042811	4.983521
C	5.597655	5.030706	4.985057
C	4.901286	6.260814	5.065890
C	5.622492	7.466372	5.217748
C	4.879999	3.805798	4.944401
C	3.458209	3.813039	4.947192
C	2.745570	5.051756	4.975864
C	3.463578	6.290283	5.036168
C	2.755863	2.575361	4.936901
C	1.326004	2.576772	4.950412
C	0.605108	3.802442	4.986272
C	1.322758	5.039594	4.977935
C	2.732796	7.515397	5.061153
C	1.320964	7.509079	4.993973
C	0.620142	6.275050	4.977575
C	2.710629	9.970251	5.094752
C	1.305878	9.970933	4.990160
C	0.599424	8.738423	4.977265
C	0.609599	11.210464	4.945861
C	1.309659	12.447018	4.933474
C	2.725005	12.434284	4.970340
C	3.407400	11.202890	5.092478
C	0.607074	1.350697	4.945013
C	5.586131	9.989310	5.703720
C	3.470252	13.663908	4.962180
C	9.866459	17.371228	4.947176
B	4.831668	8.728214	5.405721
B	4.890625	11.259796	5.302799
B	7.057428	9.945753	5.429373
Al	5.297566	10.265410	7.677571
Al	7.068550	8.897266	9.290534
Al	3.813406	9.852881	11.390749
Al	3.326613	11.507210	9.163228
Al	5.850173	11.184551	10.006141

$N_2@Al_6@BN\_graphene$

58

N	7.877987	8.530056	4.983426
N	3.515127	8.580668	5.046089
N	5.737795	12.333507	4.964316
N	4.345221	10.421982	10.000313
N	4.462267	10.380414	8.594620
C	7.152207	7.321478	4.913171
C	7.852093	6.107767	4.780542
C	9.276894	6.105173	4.764674
C	9.979229	7.345840	4.766920
C	9.268314	8.564077	4.826505
C	5.737175	7.309038	4.994365
C	5.016245	6.101691	4.850788
C	5.708671	4.869394	4.753491
C	7.128842	4.882871	4.735448
C	3.576285	6.130120	4.842767
C	2.857305	4.891684	4.775441
C	3.569987	3.649897	4.756360
C	4.989288	3.641003	4.739506
C	2.851576	7.359932	4.890886
C	1.438245	7.350842	4.811460
C	0.736999	6.115750	4.770781
C	1.436349	4.880442	4.765245
C	0.713459	8.578806	4.802430
C	1.422813	9.810174	4.846823
C	2.826746	9.811407	4.981321
C	3.523168	11.043236	5.000360
C	2.840217	12.270425	4.854562
C	1.423747	12.284314	4.784010
C	0.723616	11.048534	4.788529
C	2.869569	2.412167	4.766599
C	1.436666	2.414614	4.755848
C	0.717784	3.641365	4.761854
C	3.583040	13.503833	4.821120
C	5.012679	13.519664	4.839294
C	5.706187	14.746852	4.759082
C	7.137238	14.759070	4.736333
C	7.848432	13.534687	4.806742
C	7.147185	12.316794	4.953954
C	9.273582	13.515245	4.780417
C	9.994615	12.290563	4.780276
C	9.276086	11.069958	4.834528
C	7.875283	11.094244	4.990549
C	7.844043	15.984286	4.713987
C	9.266265	15.981170	4.737128
C	9.977270	14.748566	4.758098
C	5.717761	9.826695	5.610029
C	9.967249	9.807818	4.804937
C	9.980102	17.211099	4.750971
C	0.720690	1.190201	4.751817
B	7.174761	9.780551	5.226377
B	5.012696	11.095012	5.220044
B	4.957729	8.573263	5.272300
Al	6.020744	9.994818	7.617066
Al	5.585987	9.001894	10.139847
Al	7.756532	8.175437	8.843891

Al	7.866426	12.235163	8.214277
Al	8.148552	10.421653	10.044148
Al	5.662414	11.747557	9.660620

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C	9.951497	17.251106	4.871251
C	9.239093	16.021661	4.877254
C	7.816009	16.023605	4.866943
C	7.106075	14.806202	4.868091
C	5.676915	14.792706	4.855222
C	4.979078	13.569762	4.868667
C	3.551753	13.547850	4.860785
C	2.802122	12.316764	4.858170
C	1.389580	12.329393	4.848094
C	0.692886	11.090189	4.866215
C	1.389728	9.850236	4.879706
C	2.795915	9.850178	4.906203
C	3.486619	11.085547	4.909031
C	7.121136	12.360813	4.911520
C	7.821251	13.577978	4.881473
C	9.243344	13.559422	4.875808
C	9.948191	14.790450	4.877215
C	9.966662	12.334993	4.868070
C	9.251102	11.117912	4.873677
C	7.842621	11.144857	4.921626
C	5.676673	9.858794	5.322840
C	2.814382	7.393090	4.861474
C	1.404869	7.387744	4.862642
C	0.681707	8.617892	4.876464
C	0.707477	6.155757	4.859721
C	1.406409	4.921975	4.858212
C	2.826746	4.930580	4.852242
C	3.543433	6.167087	4.852367
C	4.982971	6.132246	4.846016
C	5.710157	7.339113	4.893333
C	7.125222	7.357420	4.891730
C	9.242954	8.605666	4.863147
C	9.938785	9.852401	4.864073
C	9.952151	7.387987	4.852647
C	9.250829	6.144507	4.865939
C	7.828388	6.141523	4.864462
C	7.100958	4.919423	4.855254
C	5.679038	4.903393	4.840470
C	4.958521	3.679718	4.843425
C	3.539069	3.690597	4.849571
C	2.837702	2.455122	4.853603
C	0.689106	1.235049	4.845204
C	1.406887	2.458725	4.852303
C	0.689279	3.683993	4.858015
N	5.707361	12.381175	4.918531
N	3.481790	8.616973	4.909690
N	7.849032	8.572155	4.924721

N	7.201940	7.556271	11.553287
N	7.900416	7.593543	10.370679
B	4.976564	11.140483	5.045190
B	4.922880	8.604185	5.040091
B	7.142665	9.828221	5.059006
Al	5.697398	9.765303	7.335807
Al	6.579571	11.114703	9.413753
Al	4.210675	9.018705	9.335357
Al	6.679472	8.005246	8.957160
Al	5.098730	10.570814	11.425603
Al	5.291337	7.929256	11.437378
Al	7.655563	9.400509	11.151032

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N	7.843386	8.586780	4.823484
N	3.476456	8.638196	4.883291
N	5.703887	12.393659	4.887002
N	4.053892	10.593463	10.808060
N	5.216526	11.346336	10.910440
C	7.123041	7.377543	4.806649
C	7.825687	6.160565	4.729802
C	9.246110	6.164129	4.710667
C	9.948913	7.406444	4.702195
C	9.231898	8.623336	4.729646
C	5.706119	7.362394	4.847111
C	4.982285	6.157081	4.746299
C	5.678187	4.924631	4.703343
C	7.098614	4.937244	4.707015
C	3.542196	6.188842	4.735403
C	2.824048	4.951316	4.703743
C	3.539720	3.709855	4.702354
C	4.958468	3.700623	4.698299
C	2.812482	7.417617	4.762135
C	1.400367	7.408229	4.715102
C	0.700207	6.173306	4.693680
C	1.402787	4.940778	4.697280
C	0.676546	8.639535	4.719593
C	1.385992	9.870353	4.751354
C	2.790161	9.869209	4.849505
C	3.485900	11.103250	4.890315
C	2.804812	12.332050	4.770630
C	1.389563	12.347497	4.715107
C	0.689487	11.111115	4.718062
C	2.839288	2.472493	4.712549
C	1.406715	2.476115	4.700669
C	0.685278	3.701263	4.697771
C	3.551725	13.562963	4.750594
C	4.980487	13.579641	4.771011
C	5.677878	14.807655	4.717530
C	7.103809	14.819534	4.716086
C	7.814459	13.589888	4.735831
C	7.110303	12.372924	4.827660

C	9.237410	13.573439	4.704765
C	9.958570	12.349301	4.698031
C	9.238441	11.131044	4.727772
C	7.832578	11.153568	4.834660
C	7.813627	16.042184	4.700436
C	9.234159	16.039802	4.701932
C	9.941910	14.807198	4.700283
C	5.680113	9.869218	5.393560
C	9.932844	9.869336	4.713328
C	9.948913	17.269361	4.702706
C	0.688920	1.252098	4.695330
B	7.131279	9.839508	5.031972
B	4.974081	11.148511	5.095243
B	4.920257	8.626268	5.064437
Al	5.912624	9.631895	7.444167
Al	7.430129	8.393103	9.042644
Al	6.608138	10.953521	9.597089
Al	4.361163	9.189825	9.526049
Al	6.000375	7.574527	11.070873
Al	7.845894	9.460757	11.391744
Al	6.383490	11.697330	12.366970
Al	4.646736	9.662408	12.361561