Electronic Supplementary Information for

Directional Diels-Alder Cycloadditions of Isoelectronic Graphene and Hexagonal-Boron Nitride in Oriented External Electric Fields: Reaction Axis Rule vs Polarization Axis Rule

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Table S1. The X,Y,Z-directional and total dipole moments (μ_X, μ_Y, μ_Z, and μ_{total}, units in D) and the amount of intermolecular charge transfer from the diene to the dienophile (Q_{CT}, units in e) in the transition states of Diels-Alder reaction between nanographene and C_2H_4 under a certain field strength along the X-axis (F_X, units in au)

F_X	μ_Z	μ_Y	μ_X	μ_{total}	Q_{CT}
-0.015	1.29	0.00	25.62	25.65	0.104
-0.010	1.18	0.00	16.87	16.91	0.100
-0.005	1.10	0.00	8.38	8.45	0.097
0	1.09	0.00	0.00	1.09	0.096
+0.005	1.10	0.00	8.38	8.45	0.097
+0.010	1.18	0.00	16.87	16.91	0.100
+0.015	1.29	0.00	25.62	25.65	0.104

Table S2. The calculated energies of reactant complex (E_{RC}, units in au), transition state (E_{TS}, units in au), reaction barrier ($E^{\ddagger}$, units in kcal mol^{-1}), and the change of barrier related to field-free condition ($\Delta E^{\ddagger}$, units in kcal mol^{-1}) of Diels-Alder reaction between nanographene and C_2H_4 under a certain field strength along the X-axis (F_X, units in au)

F_X	E_{RC}	E_{TS}	$E^{\ddagger}$	$\Delta E^{\ddagger}$
-0.015	-1689.3933	-1689.3136	50.0	3.0
-0.010	-1689.3475	-1689.2702	48.5	1.6
-0.005	-1689.3198	-1689.2445	47.2	0.3
0	-1689.3108	-1689.2360	47.0	0.0
+0.005	-1689.3198	-1689.2445	47.2	0.3
+0.010	-1689.3475	-1689.2702	48.5	1.6
+0.015	-1689.3933	-1689.3136	50.0	3.0

Table S3. The X,Y,Z-directional and total dipole moments (μ_X, μ_Y, μ_Z, and μ_{total}, units in D) and the amount of intermolecular charge transfer from the diene to the dienophile (Q_{CT}, units in e) in the transition states of Diels-Alder reaction between nanographene and C_2H_4 under a certain field strength along the Y-axis (F_Y, units in au)

F_Y	μ_Z	μ_Y	μ_X	μ_{total}	Q_{CT}
-0.015	1.04	26.43	0.00	26.45	0.101
-0.010	1.07	17.40	0.00	17.43	0.098
-0.005	1.09	8.64	0.00	8.70	0.097
0	1.09	0.00	0.00	1.09	0.096
+0.005	1.09	8.64	0.00	8.70	0.097
+0.010	1.07	17.40	0.00	17.43	0.098
+0.015	1.04	26.43	0.00	26.45	0.101

Table S4. The calculated energies of reactant complex (E_{RC}, units in au), transition state (E_{TS}, units in au), reaction barrier ($E^{\ddagger}$, units in kcal mol^{-1}), and the change of barrier related to field-free condition ($\Delta E^{\ddagger}$, units in kcal mol^{-1}) of Diels-Alder reaction between nanographene and C_2H_4 under a certain field strength along the Y-axis (F_Y, units in au)

F_Y	E_{RC}	E_{TS}	$E^{\ddagger}$	$\Delta E^{\ddagger}$
-0.015	-1689.3937	-1689.3158	48.8	1.9
-0.010	-1689.3474	-1689.2712	47.8	0.8
-0.005	-1689.3199	-1689.2448	47.1	0.2
0	-1689.3108	-1689.2360	47.0	0.0
+0.005	-1689.3199	-1689.2448	47.1	0.2
+0.010	-1689.3474	-1689.2712	47.8	0.8
+0.015	-1689.3937	-1689.3158	48.8	1.9

Table S5. The X,Y,Z-directional and total dipole moments (μ_X, μ_Y, μ_Z, and μ_{total}, units in D) and the amount of intermolecular charge transfer from the diene to the dienophile (Q_{CT}, units in e) in the transition states of Diels-Alder reaction between nanographene and C_2H_4 under a certain field strength along the Z-axis (F_Z, units in au)

F_Z	μ_Z	μ_Y	μ_X	μ_{total}	Q_{CT}
-0.015	9.95	0.00	0.00	9.95	0.236
-0.010	6.94	0.00	-0.01	6.94	0.181
-0.005	4.01	0.00	-0.01	4.01	0.139
0	1.09	0.00	0.00	1.09	0.096
+0.005	-1.90	0.00	0.01	-1.90	0.052
+0.010	-5.06	0.00	0.02	-5.06	0.007
+0.015	-8.50	0.00	0.00	-8.50	-0.044

Table S6. The calculated energies of reactant complex (E_{RC}, units in au), transition state (E_{TS}, units in au), reaction barrier ($E^{\ddagger}$, units in kcal mol^{-1}), and the change of barrier related to field-free condition ($\Delta E^{\ddagger}$, units in kcal mol^{-1}) of Diels-Alder reaction between nanographene and C_2H_4 under a certain field strength along the Z-axis (F_Z, units in au)

F_Z	E_{RC}	E_{TS}	$E^{\ddagger}$	$\Delta E^{\ddagger}$
-0.015	-1689.3349	-1689.2690	41.4	-5.6
-0.010	-1689.3214	-1689.2520	43.5	-3.4
-0.005	-1689.3134	-1689.2410	45.4	-1.6
0	-1689.3108	-1689.2360	47.0	0.0
+0.005	-1689.3134	-1689.2369	48.0	1.1
+0.010	-1689.3216	-1689.2439	48.8	1.8
+0.015	-1689.3355	-1689.2575	48.9	2.0

Table S7. The X,Y,Z-directional and total dipole moments (μ_X, μ_Y, μ_Z, and μ_{total}, units in D) and the amount of intermolecular charge transfer from the diene to the dienophile (Q_{CT}, units in e) in the transition states of Diels-Alder reaction between *h*-BN nanosheet and C_2H_4 under a certain field strength along the X-axis (F_X, units in au)

F_X	μ_Z	μ_Y	μ_X	μ_{total}	Q_{CT}
-0.015	1.35	5.29	-22.53	23.18	0.061
-0.010	1.29	5.09	-14.89	15.79	0.060
-0.005	1.24	4.97	-7.41	9.01	0.059
0	1.22	4.93	0.00	5.08	0.059
+0.005	1.24	4.97	-7.41	9.01	0.059
+0.010	1.29	5.09	-14.89	15.79	0.060
+0.015	1.35	5.29	-22.53	23.18	0.061

Table S8. The calculated energies of reactant complex (E_{RC}, units in au), transition state (E_{TS}, units in au), reaction barrier ($E^{\ddagger}$, units in kcal mol^{-1}), and the change of barrier related to field-free condition ($\Delta E^{\ddagger}$, units in kcal mol^{-1}) of Diels-Alder reaction between *h*-BN nanosheet and C_2H_4 under a certain field strength along the X-axis (F_X, units in au)

F_X	E_{RC}	E_{TS}	$E^{\ddagger}$	$\Delta E^{\ddagger}$
-0.015	-1762.8598	-1762.7640	60.1	1.0
-0.010	-1762.8208	-1762.7260	59.5	0.4
-0.005	-1762.7976	-1762.7033	59.1	0.0
0	-1762.7900	-1762.6958	59.1	0.0
+0.005	-1762.7976	-1762.7033	59.1	0.0
+0.010	-1762.8208	-1762.7260	59.5	0.4
+0.015	-1762.8598	-1762.7640	60.1	1.0

Table S9. The X,Y,Z-directional and total dipole moments (μ_X, μ_Y, μ_Z, and μ_{total}, units in D) and the amount of intermolecular charge transfer from the diene to the dienophile (Q_{CT}, units in e) in the transition states of Diels-Alder reaction between *h*-BN nanosheet and C_2H_4 under a certain field strength along the Y-axis (F_Y, units in au)

F_Y	μ_Z	μ_Y	μ_X	μ_{total}	Q_{CT}
-0.015	1.20	26.93	0.00	26.95	0.092
-0.010	1.22	19.56	0.00	19.59	0.082
-0.005	1.23	12.24	0.00	12.30	0.071
0	1.22	4.93	0.00	5.08	0.059
+0.005	1.20	-2.43	0.00	2.70	0.046
+0.010	1.14	-9.85	0.00	9.92	0.030
+0.015[a]	1.34	-14.26	0.00	14.33	0.060

a. The values were obtained based on the optimized transition state in field-free condition.

Table S10. The calculated energies of reactant complex (E_{RC}, units in au), transition state (E_{TS}, units in au), reaction barrier ($E^{\ddagger}$, units in kcal mol^{-1}), and the change of barrier related to field-free condition ($\Delta E^{\ddagger}$, units in kcal mol^{-1}) of Diels-Alder reaction between *h*-BN nanosheet and C_2H_4 under a certain field strength along the Y-axis (F_Y, units in au)

F_Y	E_{RC}	E_{TS}	$E^{\ddagger}$	$\Delta E^{\ddagger}$
-0.015	-1762.8595	-1762.7921	42.3	-16.8
-0.010	-1762.8209	-1762.7451	47.5	-11.6
-0.005	-1762.7975	-1762.7130	53.0	-6.1
0	-1762.7900	-1762.6958	59.1	0.0
+0.005	-1762.7978	-1762.6935	65.4	6.3
+0.010	-1762.8214	-1762.7063	72.3	13.2
+0.015[a]	-1762.8609	-1762.7242	85.8	26.7

a. The values were obtained based on the optimized transition state in field-free condition.

Table S11. The X,Y,Z-directional and total dipole moments (μ_X, μ_Y, μ_Z, and μ_{total}, units in D) and the amount of intermolecular charge transfer from the diene to the dienophile (Q_{CT}, units in e) in the transition states of Diels-Alder reaction between *h*-BN nanosheet and C_2H_4 under a certain field strength along the Z-axis (F_Z, units in au)

F_Z	μ_Z	μ_Y	μ_X	μ_{total}	Q_{CT}
-0.015	11.88	5.00	0.00	12.88	0.158
-0.010	8.33	4.97	0.00	9.70	0.128
-0.005	4.79	4.95	0.00	6.89	0.095
0	1.22	4.93	0.00	5.08	0.059
+0.005	-2.43	4.92	0.00	5.48	0.020
+0.010	-6.23	4.90	0.00	7.92	-0.023
+0.015	-10.29	4.88	0.00	11.38	-0.070

Table S12. The calculated energies of reactant complex (E_{RC}, units in au), transition state (E_{TS}, units in au), reaction barrier ($E^{\ddagger}$, units in kcal mol^{-1}), and the change of barrier related to field-free condition ($\Delta E^{\ddagger}$, units in kcal mol^{-1}) of Diels-Alder reaction between *h*-BN nanosheet and C_2H_4 under a certain field strength along the Z-axis (F_Z, units in au)

F_Z	E_{RC}	E_{TS}	$E^{\ddagger}$	$\Delta E^{\ddagger}$
-0.015	-1762.8203	-1762.7351	53.5	-5.6
-0.010	-1762.8034	-1762.7148	55.6	-3.5
-0.005	-1762.7933	-1762.7016	57.6	-1.5
0	-1762.7900	-1762.6958	59.1	0.0
+0.005	-1762.7929	-1762.6970	60.2	1.1
+0.010	-1762.8028	-1762.7059	60.8	1.7
+0.015	-1762.8196	-1762.7226	60.9	1.8

Table S13. The calculated NPA charge of reacting sites B and N in reactant complex (RC) and transition state (TS) and the change of local charge from RC to TS under a certain field strength along the Y-axis (F_Y, units in au)

F_Y	Q_{RC} of B	Q_{RC} of N	Q_{TS} of B	Q_{TS} of N	$Q_{TS\text{-}RC}$ of B	$Q_{TS\text{-}RC}$ of N
-0.015	1.219	-1.205	1.086	-1.118	-0.133	0.087
-0.010	1.222	-1.209	1.091	-1.126	-0.131	0.083
-0.005	1.223	-1.211	1.096	-1.133	-0.127	0.078
0	1.223	-1.212	1.100	-1.139	-0.123	0.073
+0.005	1.221	-1.211	1.103	-1.145	-0.118	0.066
+0.010	1.218	-1.208	1.104	-1.149	-0.114	0.059
+0.015	1.213	-1.204	1.104	-1.152	-0.109	0.052

Table S14. The calculated NPA charge of reacting sites B and N in reactant complex (Q_{RC}, units in e) and transition state (Q_{TS}, units in e) and the change of local charge from RC to TS ($Q_{TS\text{-}RC}$, units in e) under a certain field strength along the Z-axis (F_Z, units in au)

F_Z	Q_{RC} of B	Q_{RC} of N	Q_{TS} of B	Q_{TS} of N	$Q_{TS\text{-}RC}$ of B	$Q_{TS\text{-}RC}$ of N
-0.015	1.226	-1.214	1.086	-1.158	-0.140	0.056
-0.010	1.225	-1.213	1.091	-1.152	-0.134	0.061
-0.005	1.224	-1.213	1.096	-1.146	-0.128	0.067
0	1.223	-1.212	1.100	-1.139	-0.123	0.073
+0.005	1.222	-1.211	1.104	-1.133	-0.118	0.078
+0.010	1.220	-1.210	1.108	-1.125	-0.112	0.085
+0.015	1.218	-1.209	1.111	-1.118	-0.107	0.091

Table S15. The calculated energies of reactant complex (E_{RC}, units in au), transition state (E_{TS}, units in au), reaction barrier ($E^{\ddagger}$, units in kcal mol^{-1}), and the change of barrier related to field-free condition ($\Delta E^{\ddagger}$, units in kcal mol^{-1}) of Diels-Alder reaction between graphene nanosheet edge and C_2H_4 under a certain field strength along the Z-axis (F_Z, units in au)

F_Z	E_{RC}	E_{TS}	$E^{\ddagger}$	$\Delta E^{\ddagger}$
-0.015	-1689.3341	-1689.2760	36.5	-2.8
0	-1689.3092	-1689.2466	39.3	0.0

Table S16. The calculated energies of reactant complex (E_{RC}, units in au), transition state (E_{TS}, units in au), reaction barrier ($E^{\ddagger}$, units in kcal mol^{-1}), and the change of barrier related to field-free condition ($\Delta E^{\ddagger}$, units in kcal mol^{-1}) of Diels-Alder reaction between *h*-BN nanosheet edge and C_2H_4 under a certain field strength along the Y-axis (F_Y, units in au)

F_Y	E_{RC}	E_{TS}	$E^{\ddagger}$	$\Delta E^{\ddagger}$
-0.015	-1762.8584	-1762.8154	27.0	-17.7
0	-1762.7881	-1762.7168	44.7	0.0

Table S17. The calculated energies of reactant complex (E_{RC}, units in au), transition state (E_{TS}, units in au), reaction barrier ($E^{\ddagger}$, units in kcal mol^{-1}), and the change of barrier related to field-free condition ($\Delta E^{\ddagger}$, units in kcal mol^{-1}) of Diels-Alder reaction between graphene nanosheet and cyclopentadiene under a certain field strength along the Z-axis (F_Z, units in au)

F_Z	E_{RC}	E_{TS}	$E^{\ddagger}$	$\Delta E^{\ddagger}$
-0.015	-1804.8006	-1804.7290	45.0	-8.0
0	-1804.7730	-1804.6886	53.0	0.0
0.015	-1804.8010	-1804.7154	53.7	0.7

Table S18. The calculated energies of reactant complex (E_{RC}, units in au), transition state (E_{TS}, units in au), reaction barrier ($E^{\ddagger}$, units in kcal mol^{-1}), and the change of barrier related to field-free condition ($\Delta E^{\ddagger}$, units in kcal mol^{-1}) of Diels-Alder reaction between *h*-BN nanosheet and cyclopentadiene under a certain field strength along the Y-axis (F_Y, units in au)

F_Y	E_{RC}	E_{TS}	$E^{\ddagger}$	$\Delta E^{\ddagger}$
-0.015	-1878.3254	-1878.2109	71.9	14.5
0	-1878.2516	-1878.1601	57.4	0.0
0.015	-1878.3248	-1878.2528	45.2	-12.2

Table S19. Cartesian coordinates of optimized nanographene in field-free condition

H	-0.0018	6.7027	0.6012	C	-0.0017	1.4109	0.0012
H	-0.0024	-6.7095	0.5910	C	-2.4803	1.4286	-0.0542
C	1.1965	4.9504	0.3232	C	-4.8983	1.4535	-0.2399
C	-1.1999	4.9506	0.3211	C	-3.7075	-0.7341	-0.1525
C	-4.8941	2.8365	-0.2343	C	-1.2272	-0.7099	-0.0204
C	-2.4862	2.8436	-0.0125	C	1.2234	-0.7101	-0.0194
C	-0.0016	2.8566	0.0721	C	4.8907	-2.8420	-0.2342
C	2.4831	2.8432	-0.0080	C	2.4826	-2.8495	-0.0146
C	4.8915	2.8356	-0.2245	C	-0.0021	-2.8626	0.0677
C	3.7040	0.7284	-0.1480	C	-2.4868	-2.8491	-0.0146
C	1.2235	0.7040	-0.0181	C	-4.8950	-2.8412	-0.2334
C	-1.2270	0.7042	-0.0194	C	-1.2005	-4.9568	0.3146
C	-3.7073	0.7290	-0.1525	C	1.1960	-4.9570	0.3146
C	-4.8988	-1.4582	-0.2385	H	5.8245	3.3795	-0.3080
C	-2.4805	-1.4340	-0.0554	H	-5.8268	3.3804	-0.3207
C	-0.0020	-1.4167	-0.0010	H	-5.8279	-3.3849	-0.3185
C	2.4766	-1.4344	-0.0541	H	5.8234	-3.3858	-0.3206
C	4.8948	-1.4590	-0.2377	H	3.7202	-4.6105	-0.1367
C	3.6966	-3.5307	-0.1216	H	5.8438	-0.9502	-0.3178
C	1.2200	-3.5738	0.1235	H	5.8443	0.9439	-0.3116
C	-1.2243	-3.5736	0.1235	H	3.7215	4.6042	-0.1239
C	-3.7011	-3.5301	-0.1205	H	2.1174	5.5069	0.4183
C	-0.0023	-5.6397	0.4217	H	-2.1209	5.5072	0.4147
C	-0.0018	5.6332	0.4303	H	-3.7238	4.6048	-0.1330
C	-3.7002	3.5250	-0.1195	H	-5.8472	0.9448	-0.3216
C	-1.2238	3.5678	0.1279	H	-5.8477	-0.9493	-0.3185
C	1.2205	3.5676	0.1301	H	-3.7250	-4.6099	-0.1344
C	3.6975	3.5244	-0.1117	H	-2.1214	-5.5135	0.4080
C	3.7038	-0.7347	-0.1503	H	2.1169	-5.5137	0.4082
C	4.8953	1.4527	-0.2318	H	-0.0018	6.7027	0.6012
C	2.4769	1.4282	-0.0509	H	-0.0024	-6.7095	0.5910

Table S20. Cartesian coordinates of optimized *h*-BN nanosheet in field-free condition

H	0.0000	6.7605	0.0000	N	0.0000	1.4512	0.0000
H	0.0000	-6.9937	0.0000	N	-2.5101	1.4492	0.0000
B	1.2448	5.0688	0.0000	N	-4.9888	1.4807	0.0000
B	-1.2448	5.0688	0.0000	N	-3.7733	-0.7284	0.0000
B	-5.0255	2.9014	0.0000	N	-1.2568	-0.7256	0.0000
B	-2.5176	2.9001	0.0000	N	1.2568	-0.7256	0.0000
B	0.0000	2.9020	0.0000	N	4.9822	-2.8764	0.0000
B	2.5176	2.9001	0.0000	N	2.5175	-2.9036	0.0000
B	5.0255	2.9014	0.0000	N	0.0000	-2.8984	0.0000
B	3.7704	0.7303	0.0000	N	-2.5175	-2.9036	0.0000
B	1.2560	0.7252	0.0000	N	-4.9822	-2.8764	0.0000
B	-1.2560	0.7252	0.0000	N	-1.2121	-5.0607	0.0000
B	-3.7704	0.7303	0.0000	N	1.2121	-5.0607	0.0000
B	-5.0122	-1.4564	0.0000	H	6.0568	3.4969	0.0000
B	-2.5132	-1.4510	0.0000	H	-6.0568	3.4969	0.0000
B	0.0000	-1.4503	0.0000	H	-5.8548	-3.3803	0.0000
B	2.5132	-1.4510	0.0000	H	5.8548	-3.3803	0.0000
B	5.0122	-1.4564	0.0000	H	3.8291	-4.8007	0.0000
B	3.7674	-3.6124	0.0000	H	6.0721	-0.9156	0.0000
B	1.2528	-3.6303	0.0000	H	5.8631	0.9828	0.0000
B	-1.2528	-3.6303	0.0000	H	3.7829	4.5861	0.0000
B	-3.7674	-3.6124	0.0000	H	2.2431	5.7163	0.0000
B	0.0000	-5.8029	0.0000	H	-2.2431	5.7163	0.0000
N	0.0000	5.7528	0.0000	H	-3.7829	4.5861	0.0000
N	-3.7768	3.5800	0.0000	H	-5.8631	0.9828	0.0000
N	-1.2559	3.6320	0.0000	H	-6.0721	-0.9156	0.0000
N	1.2559	3.6320	0.0000	H	-3.8291	-4.8007	0.0000
N	3.7768	3.5800	0.0000	H	-2.0803	-5.5691	0.0000
N	3.7733	-0.7284	0.0000	H	2.0803	-5.5691	0.0000
N	4.9888	1.4807	0.0000	H	0.0000	6.7605	0.0000
N	2.5101	1.4492	0.0000	H	0.0000	-6.9937	0.0000

Table S21. Cartesian coordinates of optimized reactant complex (RC) of DA reaction between nanographene and C_2H_4 in field-free condition

H	-0.0020	6.6821	0.7088	C	-4.8970	1.4550	-0.2723
H	-0.0023	-6.6889	0.6993	C	-3.7071	-0.7341	-0.1861
C	1.1967	4.9389	0.3783	C	-1.2267	-0.7091	-0.0603
C	-1.2003	4.9391	0.3760	C	1.2229	-0.7093	-0.0593
C	-4.8922	2.8381	-0.2544	C	4.8887	-2.8436	-0.2547
C	-2.4858	2.8418	-0.0185	C	2.4821	-2.8477	-0.0207
C	-0.0016	2.8529	0.0681	C	-0.0021	-2.8589	0.0636
C	2.4826	2.8414	-0.0136	C	-2.4863	-2.8472	-0.0204
C	4.8896	2.8372	-0.2438	C	-4.8930	-2.8427	-0.2530
C	3.7036	0.7284	-0.1815	C	-1.2007	-4.9453	0.3699
C	1.2231	0.7033	-0.0581	C	1.1962	-4.9455	0.3698
C	-1.2266	0.7035	-0.0594	H	5.8219	3.3822	-0.3276
C	-3.7069	0.7290	-0.1862	H	-5.8241	3.3832	-0.3414
C	-4.8976	-1.4596	-0.2705	H	-5.8252	-3.3876	-0.3386
C	-2.4799	-1.4329	-0.0821	H	5.8206	-3.3886	-0.3417
C	-0.0019	-1.4154	-0.0352	H	3.7172	-4.6110	-0.1300
C	2.4760	-1.4333	-0.0810	H	5.8426	-0.9527	-0.3581
C	4.8936	-1.4605	-0.2702	H	5.8431	0.9463	-0.3511
C	3.6951	-3.5309	-0.1264	H	3.7187	4.6045	-0.1159
C	1.2200	-3.5685	0.1385	H	2.1181	5.4915	0.4909
C	-1.2243	-3.5683	0.1387	H	-2.1219	5.4917	0.4870
C	-3.6996	-3.5302	-0.1247	H	-3.7209	4.6053	-0.1258
C	-0.0023	-5.6247	0.4974	H	-5.8459	0.9473	-0.3618
C	-0.0019	5.6182	0.5056	H	-5.8465	-0.9516	-0.3580
C	-3.6987	3.5252	-0.1240	H	-3.7221	-4.6103	-0.1270
C	-1.2238	3.5624	0.1428	H	-2.1223	-5.4980	0.4811
C	1.2205	3.5622	0.1453	H	2.1178	-5.4982	0.4809
C	3.6961	3.5245	-0.1156	C	-0.0053	-0.6687	3.1078
C	3.7034	-0.7347	-0.1840	H	0.9167	-1.2411	3.0992
C	4.8942	1.4541	-0.2637	H	-0.9308	-1.2353	3.0991
C	2.4763	1.4271	-0.0776	C	-0.0012	0.6567	3.1090
C	-0.0017	1.4095	-0.0329	H	-0.9232	1.2289	3.1012
C	-2.4796	1.4275	-0.0810	H	0.9244	1.2232	3.1012

Table S22. Cartesian coordinates of optimized reactant complex (RC) of DA reaction between *h*-BN nanosheet and C_2H_4 in field-free condition

H	-0.00382	6.739141	0.509219	N	-4.98709	1.49671	-0.21536
H	-0.0055	-6.9388	0.56412	N	-3.7738	-0.71473	-0.17394
B	1.241173	5.063339	0.271387	N	-1.26051	-0.71095	-0.08439
B	-1.24954	5.062317	0.282726	N	1.253302	-0.71043	-0.07847
B	-5.02185	2.917463	-0.18152	N	4.971913	-2.86408	-0.14846
B	-2.52014	2.910872	-0.01658	N	2.512441	-2.88475	0.013908
B	-0.00453	2.909818	0.045322	N	-0.00361	-2.87632	0.066603
B	2.51041	2.912668	-0.03642	N	-2.51869	-2.8867	-0.01909
B	5.010289	2.920174	-0.22608	N	-4.97519	-2.86712	-0.21915
B	3.762719	0.745473	-0.16389	N	-1.21765	-5.02425	0.297497
B	1.250401	0.737949	-0.07039	N	1.208581	-5.02334	0.31334
B	-1.25872	0.737338	-0.06964	H	6.03774	3.518213	-0.29817
B	-3.77104	0.743879	-0.15986	H	-6.05072	3.515065	-0.23497
B	-5.00745	-1.44658	-0.24756	H	-5.84441	-3.37355	-0.27745
B	-2.51425	-1.43541	-0.09363	H	5.842618	-3.36998	-0.18525
B	-0.0037	-1.4315	-0.03247	H	3.817659	-4.78453	0.006342
B	2.507592	-1.43413	-0.07425	H	6.061516	-0.90531	-0.2748
B	5.002753	-1.44413	-0.19782	H	5.850206	1.002917	-0.30714
B	3.759271	-3.59622	-0.03571	H	3.767967	4.603314	-0.10375
B	1.248962	-3.60414	0.132119	H	2.242331	5.702753	0.350036
B	-1.25651	-3.60506	0.115626	H	-2.25013	5.701499	0.369961
B	-3.7634	-3.59916	-0.09634	H	-3.78038	4.600563	-0.05273
B	-0.00497	-5.7584	0.405476	H	-5.86019	1.000296	-0.27894
N	-0.004	5.740613	0.373761	H	-6.06568	-0.90808	-0.334
N	-3.77587	3.594474	-0.07852	H	-3.82012	-4.78806	-0.07042
N	-1.26079	3.637241	0.10317	H	-2.08699	-5.52842	0.352281
N	1.251634	3.638285	0.091717	H	2.077315	-5.52719	0.379077
N	3.764576	3.596968	-0.11815	C	-0.01426	-0.84435	3.141033
N	3.767123	-0.71317	-0.15315	H	0.879421	-1.45851	3.103586
N	4.977094	1.498995	-0.24114	H	-0.96275	-1.36605	3.212344
N	2.504462	1.463079	-0.08338	C	0.049833	0.478951	3.093796
N	-0.00428	1.464312	-0.05117	H	-0.84357	1.094171	3.123232
N	-2.51316	1.461831	-0.07661	H	0.998362	1.000425	3.01433

Table S23. Cartesian coordinates of optimized transition state of DA reaction between nanographene and C_2H_4 in field-free condition

H	0.0067	6.6599	0.8410	C	-4.8677	1.4685	-0.5217
H	0.0067	-6.6585	0.8401	C	-3.6828	-0.7283	-0.3894
C	1.2040	4.9139	0.5185	C	-1.2389	-0.6864	-0.0775
C	-1.1915	4.9139	0.5219	C	1.2497	-0.6864	-0.0809
C	-4.8648	2.8394	-0.3755	C	4.8748	-2.8378	-0.3896
C	-2.4804	2.8277	0.0427	C	2.4915	-2.8261	0.0354
C	0.0059	2.8236	0.3022	C	0.0059	-2.8221	0.3018
C	2.4915	2.8277	0.0358	C	-2.4804	-2.8261	0.0422
C	4.8748	2.8394	-0.3892	C	-4.8648	-2.8378	-0.3762
C	3.6928	0.7300	-0.3996	C	-1.1915	-4.9123	0.5212
C	1.2497	0.6880	-0.0808	C	1.2039	-4.9123	0.5178
C	-1.2389	0.6880	-0.0774	H	5.7979	3.3960	-0.4958
C	-3.6828	0.7300	-0.3892	H	-5.7882	3.3961	-0.4795
C	-4.8677	-1.4668	-0.5221	H	-5.7882	-3.3944	-0.4804
C	-2.4707	-1.4225	-0.1568	H	5.7978	-3.3944	-0.4962
C	0.0059	-1.3466	0.2884	H	3.7370	-4.5827	0.0382
C	2.4813	-1.4225	-0.1637	H	5.8144	-0.9694	-0.7403
C	4.8773	-1.4668	-0.5356	H	5.8144	0.9710	-0.7402
C	3.6957	-3.5103	-0.0859	H	3.7371	4.5843	0.0388
C	1.2259	-3.5307	0.3100	H	2.1249	5.4759	0.5732
C	-1.2140	-3.5307	0.3134	H	-2.1122	5.4759	0.5793
C	-3.6849	-3.5103	-0.0758	H	-3.7259	4.5843	0.0493
C	0.0064	-5.5906	0.6584	H	-5.8054	0.9710	-0.7239
C	0.0064	5.5922	0.6591	H	-5.8054	-0.9693	-0.7243
C	-3.6849	3.5119	-0.0750	H	-3.7259	-4.5827	0.0484
C	-1.2140	3.5322	0.3139	H	-2.1122	-5.4744	0.5785
C	1.2259	3.5322	0.3105	H	2.1248	-5.4744	0.5726
C	3.6957	3.5119	-0.0854	C	0.0086	-0.7132	2.1908
C	3.6928	-0.7284	-0.3996	C	0.0086	0.7145	2.1909
C	4.8773	1.4684	-0.5354	H	-0.9001	1.2193	2.5023
C	2.4813	1.4241	-0.1635	H	0.9181	1.2193	2.4998
C	0.0059	1.3481	0.2886	H	0.9181	-1.2181	2.4996
C	-2.4707	1.4241	-0.1565	H	-0.9001	-1.2181	2.5022

Table S24. Cartesian coordinates of optimized transition state of DA reaction between *h*-BN nanosheet and C_2H_4 in field-free condition

H	0.006872	6.5951	1.1445	N	-4.89165	1.5108	-0.7204
H	0.006465	-6.9375	0.6726	N	-3.72632	-0.7264	-0.4464
B	1.253257	4.9630	0.7045	N	-1.25863	-0.7232	-0.0623
B	-1.24054	4.9629	0.7075	N	1.269598	-0.7232	-0.0654
B	-4.92348	2.9237	-0.5767	N	4.946148	-2.8667	-0.3438
B	-2.49176	2.8733	0.0112	N	2.520374	-2.8771	0.1175
B	0.005995	2.8456	0.3864	N	0.006134	-2.8587	0.4442
B	2.502821	2.8733	0.0051	N	-2.5089	-2.8772	0.1236
B	4.933083	2.9238	-0.5888	N	-4.93582	-2.8668	-0.3316
B	3.72496	0.7265	-0.4897	N	-1.20781	-5.0130	0.4958
B	1.286604	0.6733	-0.0436	N	1.220259	-5.0130	0.4929
B	-1.27562	0.6733	-0.0404	H	5.931301	3.5448	-0.7769
B	-3.71507	0.7264	-0.4805	H	-5.92218	3.5447	-0.7623
B	-4.95339	-1.4661	-0.5637	H	-5.80091	-3.3788	-0.4019
B	-2.48951	-1.4501	-0.1424	H	5.81105	-3.3787	-0.4164
B	0.006186	-1.3562	0.5041	H	3.860746	-4.7473	0.2414
B	2.50029	-1.4501	-0.1485	H	5.99684	-0.9392	-0.8518
B	4.963117	-1.4660	-0.5759	H	5.757095	1.0343	-0.9661
B	3.763303	-3.5799	0.0239	H	3.745582	4.5792	-0.0733
B	1.245924	-3.5815	0.3694	H	2.25881	5.5913	0.7964
B	-1.23382	-3.5815	0.3724	H	-2.24588	5.5912	0.8019
B	-3.75205	-3.5800	0.0331	H	-3.73475	4.5791	-0.0642
B	0.006329	-5.7489	0.5726	H	-5.74838	1.0341	-0.9519
N	0.006606	5.6133	0.9157	H	-5.98782	-0.9394	-0.8370
N	-3.71512	3.5797	-0.1850	H	-3.84893	-4.7474	0.2510
N	-1.24817	3.5546	0.4030	H	-2.07575	-5.5220	0.4796
N	1.260179	3.5546	0.4000	H	2.088177	-5.5219	0.4747
N	3.725678	3.5798	-0.1942	C	0.00823	-0.7185	2.1841
N	3.736332	-0.7263	-0.4556	C	0.008179	0.7345	2.1574
N	4.900927	1.5109	-0.7324	H	-0.89435	1.2597	2.4609
N	2.488622	1.4481	-0.2075	H	0.911435	1.2597	2.4587
N	0.005982	1.3538	0.3644	H	0.911831	-1.1261	2.6346
N	-2.47805	1.4480	-0.2015	H	-0.89426	-1.1261	2.6368

Table S25. Cartesian coordinates of optimized reactant complex (RC) of DA reaction between nanographene and $C_2H_2(NO_2)_2$ in field-free condition

H	-0.0415	6.7397	-0.1049	C	-1.2256	-0.7152	-0.0668
H	0.0408	-6.7445	-0.1356	C	1.2275	-0.7039	-0.0330
C	1.1669	4.9733	-0.1432	C	4.8804	-2.7784	0.5445
C	-1.2249	4.9610	0.0217	C	2.4877	-2.8292	0.1929
C	-4.8869	2.7738	0.5304	C	0.0106	-2.8654	-0.0427
C	-2.4924	2.8239	0.1920	C	-2.4741	-2.8569	-0.1902
C	-0.0144	2.8602	-0.0341	C	-4.8891	-2.8362	-0.3263
C	2.4704	2.8512	-0.1859	C	-1.1691	-4.9789	-0.1620
C	4.8848	2.8291	-0.3315	C	1.2224	-4.9657	0.0071
C	3.7006	0.7422	-0.0458	H	5.8179	3.3659	-0.4514
C	1.2212	0.7100	-0.0523	H	-5.8122	3.2969	0.7386
C	-1.2315	0.6984	-0.0247	H	-5.8223	-3.3737	-0.4414
C	-3.7066	0.7018	0.1318	H	5.8046	-3.3012	0.7582
C	-4.8974	-1.4603	-0.1865	H	3.7212	-4.5571	0.5718
C	-2.4749	-1.4451	-0.0926	H	5.8207	-0.8737	0.4866
C	0.0043	-1.4176	-0.0375	H	5.8407	0.9354	-0.2083
C	2.4798	-1.4183	0.0857	H	3.7157	4.5969	-0.4142
C	4.8852	-1.4040	0.3842	H	2.0805	5.5459	-0.2001
C	3.6964	-3.4857	0.4370	H	-2.1484	5.5201	0.0559
C	1.2341	-3.5701	0.0569	H	-3.7280	4.5522	0.5622
C	-1.2056	-3.5840	-0.1380	H	-5.8274	0.8696	0.4705
C	-3.6915	-3.5286	-0.3129	H	-5.8456	-0.9431	-0.2052
C	0.0326	-5.6619	-0.1012	H	-3.7197	-4.6037	-0.4087
C	-0.0343	5.6569	-0.0789	H	-2.0820	-5.5519	-0.2255
C	-3.7022	3.4806	0.4288	H	2.1466	-5.5239	0.0387
C	-1.2382	3.5651	0.0615	C	-0.0989	-0.6597	2.9287
C	1.2021	3.5784	-0.1301	C	0.0956	0.6455	2.9311
C	3.6877	3.5221	-0.3150	N	1.4678	1.1591	2.9109
C	3.7017	-0.7072	0.1374	N	-1.4710	-1.1735	2.9046
C	4.8930	1.4535	-0.1879	O	-2.3837	-0.3779	2.9281
C	2.4706	1.4392	-0.0934	O	-1.5753	-2.3781	2.8543
C	-0.0089	1.4126	-0.0480	O	1.5724	2.3638	2.8626
C	-2.4848	1.4132	0.0800	O	2.3805	0.3634	2.9348
C	-4.8911	1.3993	0.3721	H	0.6691	-1.4192	2.9174
C	-3.7050	-0.7479	-0.0497	H	-0.6722	1.4053	2.9202

Table S26. Cartesian coordinates of optimized transition state of DA reaction between nanographene and $C_2H_2(NO_2)_2$ in field-free condition

H	0.0385	6.6757	0.6907	C	-1.2458	-0.6786	-0.0975
H	-0.0254	-6.6741	0.6917	C	1.2551	-0.6915	-0.0726
C	1.2183	4.9238	0.3461	C	4.9071	-2.8080	-0.0064
C	-1.1725	4.9197	0.5142	C	2.4947	-2.8166	0.1901
C	-4.8963	2.8095	0.0100	C	-0.0041	-2.8288	0.2742
C	-2.4832	2.8181	0.1983	C	-2.4738	-2.8273	-0.1298
C	0.0158	2.8304	0.2740	C	-4.8348	-2.8218	-0.6593
C	2.4842	2.8288	-0.1382	C	-1.2063	-4.9222	0.3506
C	4.8434	2.8233	-0.6757	C	1.1850	-4.9181	0.5108
C	3.6887	0.7135	-0.4508	H	5.7520	3.3777	-0.8760
C	1.2563	0.6801	-0.1017	H	-5.8339	3.3498	0.0551
C	-1.2444	0.6930	-0.0685	H	-5.7440	-3.3763	-0.8566
C	-3.6925	0.7365	-0.2964	H	5.8448	-3.3483	0.0355
C	-4.8502	-1.4444	-0.6851	H	3.7609	-4.5345	0.4710
C	-2.4702	-1.4156	-0.2355	H	5.8488	-0.9561	-0.4333
C	-0.0022	-1.3505	0.2851	H	5.7884	0.9384	-0.9156
C	2.4881	-1.4270	-0.0889	H	3.7078	4.5887	-0.3260
C	4.9040	-1.4578	-0.2819	H	2.1396	5.4868	0.3314
C	3.7142	-3.4804	0.2397	H	-2.0886	5.4850	0.6001
C	1.2160	-3.5306	0.3572	H	-3.7485	4.5360	0.4836
C	-1.2198	-3.5366	0.1820	H	-5.8394	0.9575	-0.4137
C	-3.6625	-3.5084	-0.3551	H	-5.7806	-0.9370	-0.8961
C	-0.0175	-5.6009	0.5460	H	-3.6980	-4.5872	-0.3134
C	0.0301	5.6025	0.5453	H	-2.1277	-5.4852	0.3391
C	-3.7026	3.4819	0.2521	H	2.1014	-5.4834	0.5938
C	-1.2039	3.5321	0.3609	C	0.0042	-0.7189	2.1461
C	1.2312	3.5382	0.1777	C	0.0139	0.7206	2.1460
C	3.6721	3.5099	-0.3675	H	-0.8554	1.2397	2.5280
C	3.7024	-0.7350	-0.3088	H	0.8748	-1.2380	2.5252
C	4.8587	1.4459	-0.7014	N	1.2422	1.3232	2.6803
C	2.4802	1.4171	-0.2439	N	-1.2223	-1.3214	2.6845
C	0.0140	1.3520	0.2851	O	1.1548	2.4714	3.0597
C	-2.4776	1.4285	-0.0807	O	2.2647	0.6651	2.6667
C	-4.8941	1.4593	-0.2655	O	-2.2448	-0.6633	2.6742
C	-3.6794	-0.7120	-0.4385	O	-1.1336	-2.4696	3.0637

Table S27. Cartesian coordinates of optimized reactant complex (RC) of DA reaction between nanographene (at edge) and C_2H_4 in field-free condition

H	0.0980	6.7660	-0.0681	C	-4.7896	1.4372	-0.1062
H	0.1495	-6.7243	0.0858	C	-3.5796	-0.7173	0.1999
C	1.3006	4.9955	-0.0230	C	-1.1033	-0.6908	0.0404
C	-1.0952	4.9888	-0.0780	C	1.3421	-0.6826	-0.0860
C	-4.7948	2.8133	-0.2472	C	5.0018	-2.7729	-0.5888
C	-2.3791	2.8542	-0.1125	C	2.6036	-2.8143	-0.2612
C	0.1079	2.8832	-0.0366	C	0.1291	-2.8421	0.0058
C	2.5949	2.8695	0.0526	C	-2.3469	-2.8287	0.2597
C	5.0078	2.8385	0.2323	C	-4.7482	-2.8035	0.5581
C	3.8191	0.7582	-0.0859	C	-1.0523	-4.9546	0.1619
C	1.3382	0.7320	-0.0687	C	1.3327	-4.9471	-0.0691
C	-1.1092	0.7237	0.0074	H	5.9403	3.3697	0.3787
C	-3.5906	0.7346	0.0283	H	-5.7328	3.3417	-0.3662
C	-4.7617	-1.4275	0.4175	H	-5.6724	-3.3381	0.7405
C	-2.3500	-1.4170	0.1552	H	5.9288	-3.3030	-0.7702
C	0.1222	-1.3945	-0.0136	H	3.8479	-4.5532	-0.5499
C	2.5946	-1.4005	-0.1938	H	5.9397	-0.8654	-0.5876
C	5.0034	-1.3937	-0.4807	H	5.9556	0.9391	0.1230
C	3.8170	-3.4770	-0.4639	H	3.8405	4.6084	0.3265
C	1.3490	-3.5516	-0.1110	H	2.2195	5.5632	-0.0258
C	-1.0841	-3.5586	0.1461	H	-2.0161	5.5530	-0.0875
C	-3.5553	-3.4976	0.4677	H	-3.6388	4.5890	-0.3490
C	0.1438	-5.6415	0.0618	H	-5.7333	0.9119	-0.1279
C	0.1009	5.6829	-0.0573	H	-5.7049	-0.9081	0.5042
C	-3.6031	3.5153	-0.2376	H	-3.5771	-4.5714	0.5802
C	-1.1166	3.5925	-0.0801	H	-1.9654	-5.5247	0.2484
C	1.3286	3.5997	0.0021	H	2.2523	-5.5098	-0.1310
C	3.8131	3.5357	0.2034	C	4.0925	-1.5378	3.0267
C	3.8173	-0.6916	-0.2622	H	4.8913	-1.7585	3.7264
C	5.0122	1.4637	0.0789	H	3.9308	-2.2513	2.2246
C	2.5903	1.4582	-0.0521	C	3.3484	-0.4478	3.1472
C	0.1119	1.4355	-0.0326	H	2.5454	-0.2270	2.4511
C	-2.3657	1.4422	-0.0125	H	3.5088	0.2654	3.9482

Table S28. Cartesian coordinates of optimized transition state of DA reaction between nanographene (at edge) and C_2H_4 in field-free condition

H	-0.1311	6.7007	0.6480	C	-5.0070	1.4526	-0.3930
H	-0.0896	-6.6846	0.6503	C	-3.8141	-0.7352	-0.2645
C	1.0751	4.9503	0.4282	C	-1.3441	-0.6999	-0.0506
C	-1.3234	4.9513	0.3136	C	1.1047	-0.6964	0.0042
C	-5.0019	2.8352	-0.3873	C	4.8134	-2.7914	0.0972
C	-2.6025	2.8477	-0.0810	C	2.3781	-2.8035	0.1575
C	-0.1194	2.8588	0.1037	C	-0.1017	-2.8427	0.1054
C	2.3606	2.8351	0.1549	C	-2.5848	-2.8471	-0.0800
C	4.7959	2.8381	0.0935	C	-4.9841	-2.8497	-0.3868
C	3.5760	0.7201	-0.0806	C	-1.2927	-4.9427	0.3153
C	1.1003	0.7199	0.0036	C	1.1057	-4.9267	0.4307
C	-1.3484	0.7082	-0.0511	H	5.7338	3.3816	0.0752
C	-3.8187	0.7281	-0.2647	H	-5.9311	3.3793	-0.5053
C	-4.9978	-1.4672	-0.3930	H	-5.9099	-3.3996	-0.5049
C	-2.5888	-1.4309	-0.1241	H	5.7547	-3.3291	0.0801
C	-0.1138	-1.4068	0.0092	H	3.6790	-4.5518	0.2092
C	2.3551	-1.4131	0.0315	H	5.7010	-0.9160	-0.4124
C	4.8303	-1.3592	0.0556	H	5.6951	0.9676	-0.4137
C	3.6439	-3.4722	0.1749	H	3.6505	4.5915	0.2038
C	1.1307	-3.5380	0.2342	H	1.9912	5.5064	0.5631
C	-1.3222	-3.5649	0.1138	H	-2.2448	5.5130	0.3681
C	-3.7903	-3.5333	-0.2296	H	-3.8370	4.6063	-0.2432
C	-0.0891	-5.6147	0.4803	H	-5.9525	0.9433	-0.5068
C	-0.1239	5.6309	0.4781	H	-5.9465	-0.9638	-0.5074
C	-3.8123	3.5263	-0.2307	H	-3.8083	-4.6135	-0.2418
C	-1.3444	3.5733	0.1123	H	-2.2106	-5.5101	0.3696
C	1.1086	3.5618	0.2319	H	2.0252	-5.4771	0.5659
C	3.6222	3.5117	0.1710	C	5.4539	-0.6784	1.8746
C	3.5803	-0.6812	-0.0798	C	5.4494	0.7316	1.8737
C	4.8217	1.4060	0.0538	H	6.4115	-1.1861	1.8553
C	2.3462	1.4444	0.0302	H	4.6819	-1.1996	2.4274
C	-0.1226	1.4228	0.0085	H	6.4038	1.2455	1.8537
C	-2.5977	1.4314	-0.1246	H	4.6740	1.2487	2.4256

Table S29. Cartesian coordinates of optimized reactant complex (RC) of DA reaction between h-BN nanosheet (at edge) and C_2H_4 in field-free condition

H	-0.0800	6.8308	0.1416	N	-4.9794	1.4756	-0.2219
H	0.1478	-6.8870	0.5291	N	-3.7360	-0.7085	-0.0045
B	1.1920	5.1594	0.0957	N	-1.2212	-0.6666	0.0215
B	-1.2973	5.1227	0.0222	N	1.2894	-0.6292	-0.0340
B	-5.0336	2.8941	-0.2997	N	5.0288	-2.7265	-0.3437
B	-2.5330	2.9362	-0.1220	N	2.5817	-2.7876	-0.0556
B	-0.0186	2.9774	-0.0123	N	0.0702	-2.8164	0.1110
B	2.4991	3.0107	0.0182	N	-2.4459	-2.8593	0.1641
B	5.0073	3.0401	0.0292	N	-4.9110	-2.8708	0.1415
B	3.7797	0.8583	-0.1112	N	-1.1012	-4.9849	0.3633
B	1.2677	0.8203	-0.0401	N	1.3228	-4.9498	0.2605
B	-1.2422	0.7826	-0.0271	H	6.0308	3.6472	0.0778
B	-3.7536	0.7469	-0.1031	H	-6.0701	3.4710	-0.4059
B	-4.9629	-1.4544	0.0413	H	-5.7757	-3.3873	0.1701
B	-2.4656	-1.4102	0.0602	H	5.9028	-3.2173	-0.4471
B	0.0458	-1.3715	0.0305	H	3.9053	-4.6679	-0.2139
B	2.5546	-1.3351	-0.1003	H	6.0866	-0.7462	-0.4385
B	5.0418	-1.3042	-0.3247	H	5.8675	1.1300	-0.0677
B	3.8333	-3.4795	-0.2018	H	3.7441	4.7094	0.1113
B	1.3347	-3.5274	0.1054	H	2.1804	5.8208	0.1473
B	-1.1690	-3.5631	0.2153	H	-2.3072	5.7529	0.0254
B	-3.6846	-3.5859	0.2010	H	-3.8170	4.5996	-0.2916
B	0.1250	-5.7038	0.3960	H	-5.8451	0.9635	-0.2535
N	-0.0637	5.8243	0.0943	H	-6.0310	-0.9303	0.0024
N	-3.7977	3.5946	-0.2427	H	-3.7266	-4.7731	0.2764
N	-1.2852	3.6877	-0.0419	H	-1.9592	-5.5034	0.4507
N	1.2268	3.7243	0.0375	H	2.2008	-5.4416	0.2760
N	3.7501	3.7044	0.0585	C	4.8153	-1.4133	2.9709
N	3.7971	-0.5953	-0.2030	H	5.6318	-2.0021	3.3741
N	4.9890	1.6217	-0.0591	H	4.0131	-1.9581	2.4833
N	2.5113	1.5614	-0.0464	C	4.7950	-0.0914	3.0672
N	0.0023	1.5276	-0.0285	H	3.9748	0.4943	2.6653
N	-2.5057	1.4864	-0.0782	H	5.5932	0.4588	3.5529

Table S30. Cartesian coordinates of optimized transition state of DA reaction between h-BN nanosheet (at edge) and C_2H_4 in field-free condition

H	-0.1311	6.7007	0.6480	C	-5.0070	1.4526	-0.3930
H	-0.0896	-6.6846	0.6503	C	-3.8141	-0.7352	-0.2645
C	1.0751	4.9503	0.4282	C	-1.3441	-0.6999	-0.0506
C	-1.3234	4.9513	0.3136	C	1.1047	-0.6964	0.0042
C	-5.0019	2.8352	-0.3873	C	4.8134	-2.7914	0.0972
C	-2.6025	2.8477	-0.0810	C	2.3781	-2.8035	0.1575
C	-0.1194	2.8588	0.1037	C	-0.1017	-2.8427	0.1054
C	2.3606	2.8351	0.1549	C	-2.5848	-2.8471	-0.0800
C	4.7959	2.8381	0.0935	C	-4.9841	-2.8497	-0.3868
C	3.5760	0.7201	-0.0806	C	-1.2927	-4.9427	0.3153
C	1.1003	0.7199	0.0036	C	1.1057	-4.9267	0.4307
C	-1.3484	0.7082	-0.0511	H	5.7338	3.3816	0.0752
C	-3.8187	0.7281	-0.2647	H	-5.9311	3.3793	-0.5053
C	-4.9978	-1.4672	-0.3930	H	-5.9099	-3.3996	-0.5049
C	-2.5888	-1.4309	-0.1241	H	5.7547	-3.3291	0.0801
C	-0.1138	-1.4068	0.0092	H	3.6790	-4.5518	0.2092
C	2.3551	-1.4131	0.0315	H	5.7010	-0.9160	-0.4124
C	4.8303	-1.3592	0.0556	H	5.6951	0.9676	-0.4137
C	3.6439	-3.4722	0.1749	H	3.6505	4.5915	0.2038
C	1.1307	-3.5380	0.2342	H	1.9912	5.5064	0.5631
C	-1.3222	-3.5649	0.1138	H	-2.2448	5.5130	0.3681
C	-3.7903	-3.5333	-0.2296	H	-3.8370	4.6063	-0.2432
C	-0.0891	-5.6147	0.4803	H	-5.9525	0.9433	-0.5068
C	-0.1239	5.6309	0.4781	H	-5.9465	-0.9638	-0.5074
C	-3.8123	3.5263	-0.2307	H	-3.8083	-4.6135	-0.2418
C	-1.3444	3.5733	0.1123	H	-2.2106	-5.5101	0.3696
C	1.1086	3.5618	0.2319	H	2.0252	-5.4771	0.5659
C	3.6222	3.5117	0.1710	C	5.4539	-0.6784	1.8746
C	3.5803	-0.6812	-0.0798	C	5.4494	0.7316	1.8737
C	4.8217	1.4060	0.0538	H	6.4115	-1.1861	1.8553
C	2.3462	1.4444	0.0302	H	4.6819	-1.1996	2.4274
C	-0.1226	1.4228	0.0085	H	6.4038	1.2455	1.8537
C	-2.5977	1.4314	-0.1246	H	4.6740	1.2487	2.4256

Table S31. Cartesian coordinates of optimized reactant complex (RC) of DA reaction between nanographene and cyclopentadiene in field-free condition

H	-0.0962	6.5521	0.8683	C	1.2658	-0.7893	-0.0941
H	0.1521	-6.8083	0.4945	C	4.9565	-2.8535	-0.4559
C	1.1390	4.8420	0.5007	C	2.5579	-2.9064	-0.1573
C	-1.2574	4.8050	0.4373	C	0.0761	-2.9616	-0.0190
C	-4.8988	2.6630	-0.3211	C	-2.4105	-2.9865	-0.0450
C	-2.4967	2.7017	-0.0528	C	-4.8252	-3.0140	-0.1751
C	-0.0174	2.7507	0.0911	C	-1.0808	-5.0752	0.2491
C	2.4677	2.7789	0.0636	C	1.3154	-5.0356	0.1960
C	4.8790	2.8174	-0.1126	H	5.8048	3.3783	-0.1492
C	3.7233	0.6919	-0.1694	H	-5.8369	3.1939	-0.4277
C	1.2431	0.6242	-0.0615	H	-5.7534	-3.5712	-0.2079
C	-1.2064	0.5842	-0.0797	H	5.8929	-3.3791	-0.5981
C	-3.6840	0.5716	-0.2200	H	3.8141	-4.6433	-0.3815
C	-4.8475	-1.6314	-0.2156	H	5.8794	-0.9444	-0.5017
C	-2.4258	-1.5728	-0.1120	H	5.8631	0.9453	-0.2711
C	0.0517	-1.5160	-0.0837	H	3.6786	4.5619	0.0546
C	2.5302	-1.4913	-0.1554	H	2.0483	5.4046	0.6554
C	4.9417	-1.4712	-0.4041	H	-2.1914	5.3373	0.5465
C	3.7772	-3.5650	-0.3257	H	-3.7524	4.4481	-0.1873
C	1.3110	-3.6524	0.0057	H	-5.8235	0.7576	-0.4302
C	-1.1333	-3.6918	0.0637	H	-5.8057	-1.1357	-0.2655
C	-3.6189	-3.6850	-0.0919	H	-3.6303	-4.7650	-0.0758
C	0.1310	-5.7382	0.3281	H	-1.9893	-5.6494	0.3569
C	-0.0735	5.4971	0.6241	H	2.2486	-5.5750	0.2710
C	-3.7168	3.3681	-0.1783	C	-0.4650	0.1071	3.2543
C	-1.2518	3.4379	0.1535	H	0.2315	-0.1583	2.4491
C	1.1908	3.4749	0.2189	H	0.0383	-0.1503	4.1943
C	3.6724	3.4824	0.0130	C	-0.8551	1.5573	3.2156
C	3.7443	-0.7691	-0.2486	H	-0.1503	2.3767	3.2671
C	4.9047	1.4366	-0.1912	C	-2.1894	1.6539	3.1008
C	2.4850	1.3680	-0.0517	H	-2.7616	2.5709	3.0405
C	0.0066	1.3097	-0.0362	C	-1.7818	-0.6030	3.1216
C	-2.4689	1.2885	-0.1152	H	-1.8879	-1.6793	3.0887
C	-4.8838	1.2796	-0.3265	C	-2.7689	0.3035	3.0412
C	-3.6638	-0.8910	-0.1912	H	-3.8246	0.0913	2.9310
C	-1.1841	-0.8291	-0.0953				

Table S32. Cartesian coordinates of optimized transition state of DA reaction between nanographene and cyclopentadiene in field-free condition

H	0.0531	6.7278	0.6163	C	1.2366	-0.7207	0.0178
H	0.0850	-6.7077	0.6760	C	4.8178	-2.8329	-0.8582
C	1.2490	4.9853	0.3060	C	2.4817	-2.8507	-0.2397
C	-1.1501	4.9598	0.3974	C	0.0457	-2.8600	0.1737
C	-4.7409	2.8150	-0.6435	C	-2.4431	-2.8435	0.2032
C	-2.4140	2.8451	-0.0046	C	-4.8388	-2.8329	-0.1016
C	0.0629	2.8736	0.1726	C	-1.1358	-4.9466	0.5233
C	2.5221	2.8577	-0.0399	C	1.2467	-4.9689	0.2365
C	4.9215	2.8273	-0.3333	H	5.8650	3.3547	-0.4023
C	3.6981	0.7365	-0.3619	H	-5.6315	3.3365	-0.9720
C	1.2388	0.7322	0.0247	H	-5.7715	-3.3707	-0.2195
C	-1.1936	0.7559	0.6079	H	5.7194	-3.3653	-1.1354
C	-3.6183	0.7383	-0.0872	H	3.6783	-4.6075	-0.6218
C	-4.8315	-1.4497	-0.0976	H	5.7401	-0.9266	-1.0453
C	-2.4375	-1.4352	0.2321	H	5.8314	0.9202	-0.5644
C	0.0531	-1.4149	0.2050	H	3.7939	4.6046	-0.0836
C	2.4699	-1.4361	-0.2304	H	2.1678	5.5532	0.3291
C	4.8228	-1.4439	-0.8047	H	-2.0798	5.5040	0.4977
C	3.6662	-3.5285	-0.5631	H	-3.5463	4.5825	-0.5789
C	1.2559	-3.5762	0.0532	H	-5.6766	0.9125	-0.7092
C	-1.1725	-3.5726	0.3266	H	-5.7733	-0.9303	-0.2008
C	-3.6453	-3.5257	0.0150	H	-3.6552	-4.6046	-0.0560
C	0.0721	-5.6390	0.5002	H	-2.0490	-5.4955	0.7083
C	0.0559	5.6557	0.4621	H	2.1710	-5.5280	0.2092
C	-3.5700	3.5144	-0.4091	C	-0.2595	0.0526	2.9045
C	-1.1633	3.5852	0.2161	H	-0.0795	0.1170	3.9839
C	1.2789	3.5887	0.1473	H	0.6994	0.0524	2.3926
C	3.7508	3.5269	-0.1445	C	-1.1515	-1.1237	2.6277
C	3.6759	-0.7305	-0.4745	H	-0.8166	-2.1518	2.7017
C	4.8940	1.4417	-0.4368	C	-2.4640	-0.7037	2.9856
C	2.4893	1.4460	-0.1430	H	-3.3164	-1.3599	3.1039
C	0.0608	1.4310	0.2072	C	-1.2224	1.1468	2.5089
C	-2.4281	1.4466	0.1384	H	-0.9579	2.1960	2.5856
C	-4.7612	1.4408	-0.4851	C	-2.5102	0.6675	2.9243
C	-3.6378	-0.7320	0.0323	H	-3.4037	1.2740	2.9925
C	-1.1863	-0.7314	0.5832				

Table S33. Cartesian coordinates of optimized reactant complex (RC) of DA reaction between h-BN nanosheet and cyclopentadiene in field-free condition

H	0.1177	6.8683	0.1944	N	1.3090	-0.6138	-0.0424
H	-0.0027	-6.8083	0.7740	N	5.0131	-2.7956	-0.0457
B	1.3445	5.1720	0.0179	N	2.5528	-2.7948	0.1011
B	-1.1442	5.1899	0.1198	N	0.0371	-2.7696	0.1197
B	-4.9456	3.0495	0.0427	N	-2.4748	-2.7667	-0.0161
B	-2.4387	3.0335	-0.0019	N	-4.9299	-2.7293	-0.2106
B	0.0788	3.0188	-0.0393	N	-1.1971	-4.8978	0.4134
B	2.5909	2.9980	-0.2011	N	1.2293	-4.9127	0.4653
B	5.0853	2.9751	-0.4534	H	6.1144	3.5601	-0.5841
B	3.8264	0.8168	-0.2415	H	-5.9733	3.6501	0.0870
B	1.3171	0.8357	-0.0947	H	-5.8017	-3.2287	-0.2881
B	-1.1949	0.8525	-0.0583	H	5.8808	-3.3078	-0.0568
B	-3.7033	0.8731	-0.0677	H	3.8443	-4.7022	0.1691
B	-4.9535	-1.3077	-0.2026	H	6.1155	-0.8506	-0.2508
B	-2.4611	-1.3141	-0.0547	H	5.9110	1.0497	-0.4516
B	0.0447	-1.3276	-0.0010	H	3.8581	4.6721	-0.3903
B	2.5591	-1.3483	-0.0325	H	2.3510	5.8078	0.0216
B	5.0531	-1.3795	-0.1571	H	-2.1360	5.8438	0.1971
B	3.7949	-3.5158	0.0847	H	-3.6929	4.7278	0.0775
B	1.2827	-3.5018	0.2300	H	-5.7949	1.1338	0.0025
B	-1.2232	-3.4863	0.1716	H	-6.0083	-0.7603	-0.2800
B	-3.7205	-3.4709	-0.1134	H	-3.7797	-4.6604	-0.1240
B	0.0085	-5.6352	0.5680	H	-2.0717	-5.3926	0.4732
N	0.1076	5.8631	0.1238	H	2.0930	-5.4199	0.5636
N	-3.6935	3.7223	0.0394	C	-0.3868	-0.4370	3.2937
N	-1.1706	3.7568	0.0293	H	0.1562	-0.3876	4.2457
N	1.3407	3.7387	-0.0771	H	0.3751	-0.4127	2.5047
N	3.8473	3.6665	-0.3509	C	-1.2520	-1.6621	3.2207
N	3.8217	-0.6394	-0.1499	H	-0.8742	-2.6747	3.2679
N	5.0430	1.5553	-0.3899	C	-2.5368	-1.2893	3.0961
N	2.5750	1.5476	-0.1729	H	-3.3904	-1.9508	3.0207
N	0.0681	1.5697	-0.0640	C	-1.3744	0.6863	3.1661
N	-2.4421	1.5873	-0.0724	H	-1.1039	1.7337	3.1644
N	-4.9185	1.6287	-0.0037	C	-2.6131	0.1776	3.0596
N	-3.7164	-0.5847	-0.1132	H	-3.5295	0.7443	2.9513
N	-1.2021	-0.5960	-0.0540				

Table S34. Cartesian coordinates of optimized transition state of DA reaction between h-BN nanosheet and cyclopentadiene in field-free condition

H	0.0383	6.7724	0.4019	N	1.2913	-0.6812	-0.1741
H	0.1142	-6.9448	0.1821	N	4.9241	-2.8052	-1.1004
B	1.2967	5.1118	0.1278	N	2.5359	-2.8500	-0.4988
B	-1.1977	5.0808	0.1791	N	0.0620	-2.8592	-0.0736
B	-4.7472	2.8787	-1.1825	N	-2.4458	-2.8844	-0.0072
B	-2.4080	2.9103	-0.2925	N	-4.8855	-2.8392	-0.3084
B	0.0746	2.9348	0.0284	N	-1.1220	-5.0256	0.1658
B	2.5635	2.9565	-0.2405	N	1.2861	-5.0133	-0.1353
B	5.0431	2.9542	-0.6134	H	6.0735	3.5429	-0.7203
B	3.7705	0.7933	-0.5996	H	-5.6986	3.4435	-1.6271
B	1.2870	0.7932	-0.1443	H	-5.7618	-3.3289	-0.3965
B	-1.2227	0.8482	0.5463	H	5.7687	-3.2983	-1.3429
B	-3.5976	0.7627	-0.4922	H	3.7984	-4.7380	-0.8879
B	-4.8778	-1.4209	-0.4491	H	5.9791	-0.8332	-1.2905
B	-2.4444	-1.4338	0.0005	H	5.8453	1.0393	-0.8960
B	0.0743	-1.4150	0.0243	H	3.8336	4.6372	-0.2976
B	2.5249	-1.3947	-0.4655	H	2.2923	5.7676	0.1444
B	4.9530	-1.3837	-1.0451	H	-2.2147	5.7028	0.2263
B	3.7491	-3.5501	-0.8262	H	-3.5464	4.5818	-0.9142
B	1.3099	-3.5849	-0.2406	H	-5.5467	0.9438	-1.3098
B	-1.1799	-3.6049	0.0400	H	-5.9109	-0.8657	-0.6464
B	-3.6933	-3.5892	-0.1459	H	-3.7530	-4.7779	-0.1302
B	0.0970	-5.7589	0.0827	H	-1.9824	-5.5355	0.2810
N	0.0463	5.7721	0.2824	H	2.1551	-5.5146	-0.2183
N	-3.5770	3.5825	-0.7925	C	-0.3720	-0.0566	2.7234
N	-1.1897	3.6595	0.0299	H	-0.2708	-0.0846	3.8136
N	1.3235	3.6851	-0.0318	H	0.6167	-0.0523	2.2680
N	3.8211	3.6330	-0.3686	C	-1.2537	-1.1939	2.3002
N	3.7557	-0.6672	-0.7084	H	-0.9219	-2.2268	2.2980
N	4.9869	1.5363	-0.7277	C	-2.5968	-0.8108	2.6955
N	2.5404	1.5056	-0.3439	H	-3.4389	-1.4835	2.7767
N	0.0808	1.4996	0.0873	C	-1.3130	1.0708	2.2786
N	-2.4286	1.4844	-0.1365	H	-1.0724	2.0912	2.5704
N	-4.7334	1.4631	-1.0247	C	-2.6193	0.5481	2.6781
N	-3.6381	-0.7076	-0.3225	H	-3.5069	1.1563	2.8091
N	-1.1950	-0.7379	0.4352				

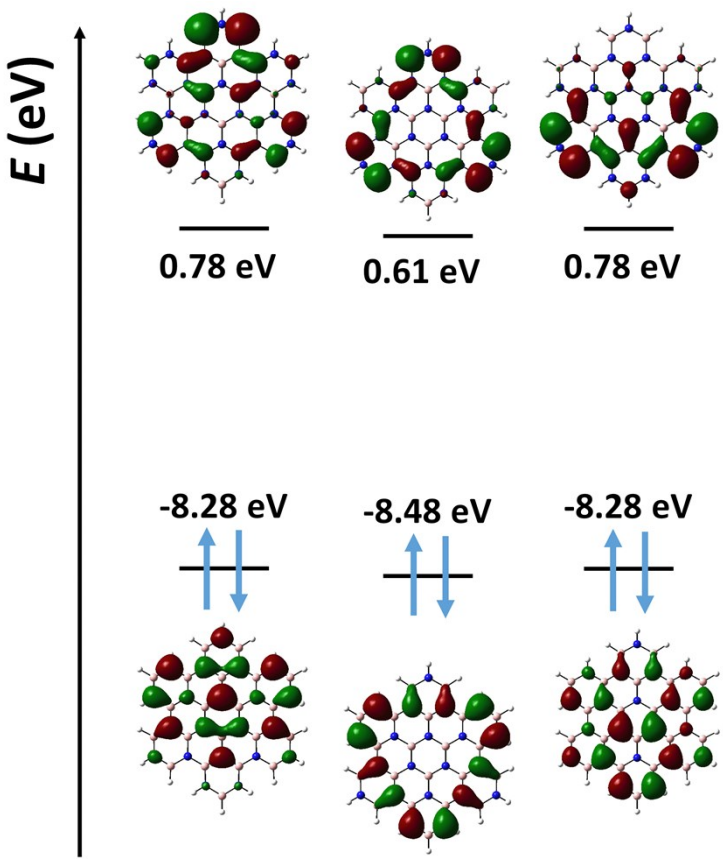

Figure S1. Frontier molecular orbital diagrams of h-BN nanosheet.

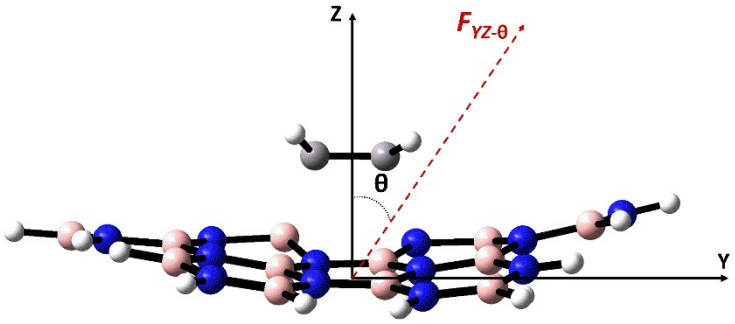

Figure S2. Definition of the 2-D field $F_{YZ\text{-}\theta}$.

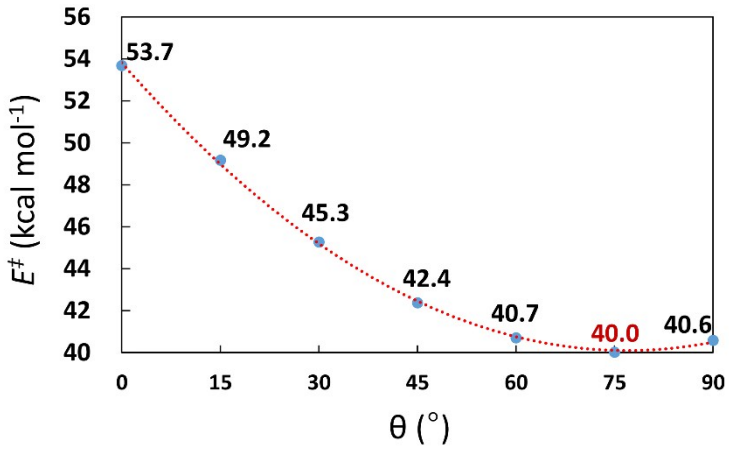

Figure S3. Plots of barriers ($E^{\ddagger}$) of the DA reaction between h-BN nanosheet and C_2H_4 versus the angle θ of the 2-D field $F_{YZ\text{-}\theta}$ with the strength of -0.015 au.

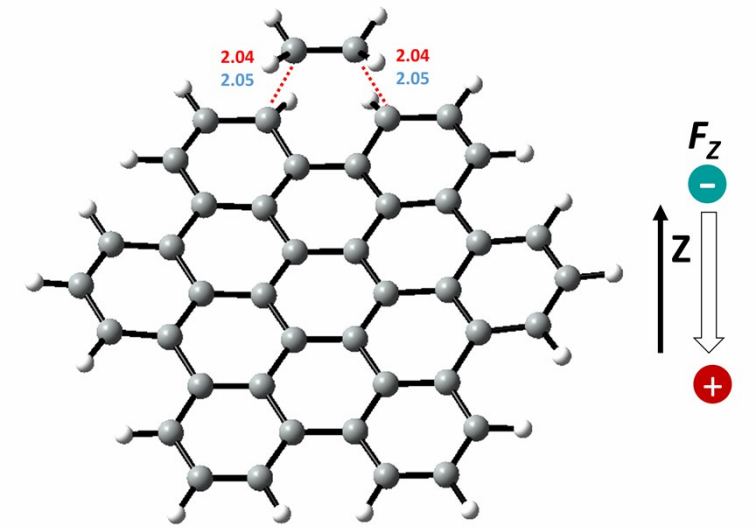

Figure S4. Transition state structures of DA reaction between nanographene (at edge) and C_2H_4 in field-free (red) and F_Z = -0.015 au (blue) conditions.

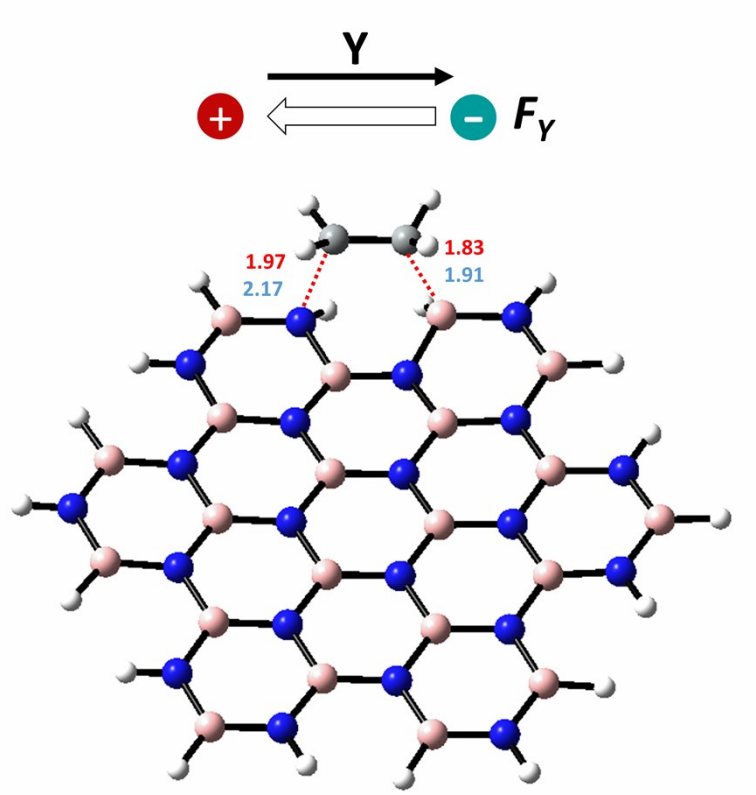

Figure S5. Transition state structures of DA reaction between h-BN nanosheet (at edge) and C_2H_4 in field-free (red) and F_Y = -0.015 au (blue) conditions.

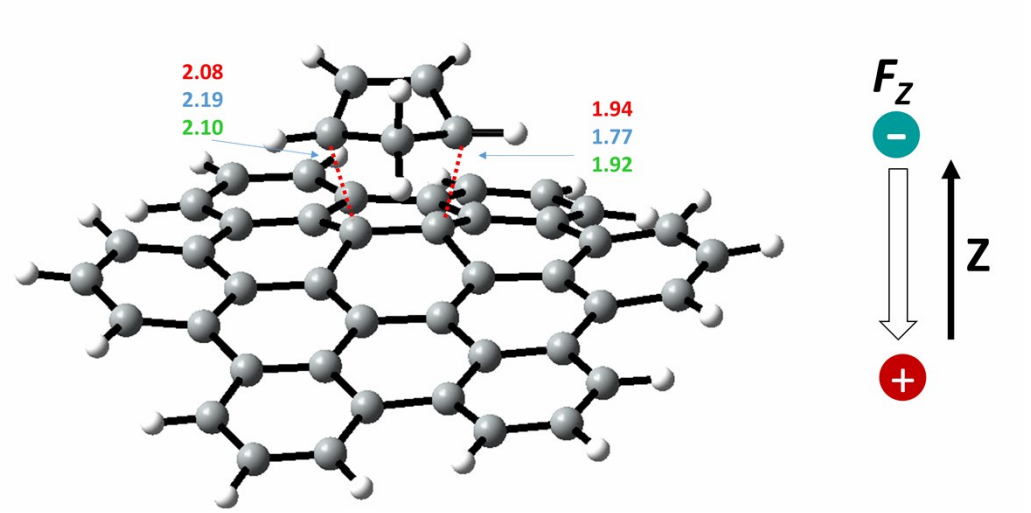

Figure S6. Transition state structures of DA reaction between nanographene and cyclopentadiene in field-free (red), F_Z = -0.015 au (blue), and F_Z = +0.015 au (green) conditions.

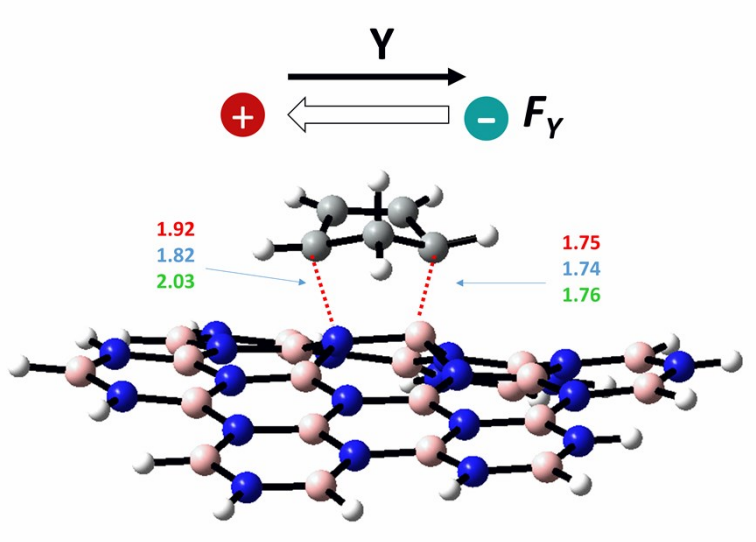

Figure S7. Transition state structures of DA reaction between h-BN nanosheet and cyclopentadiene in field-free (red), F_Y = -0.015 au (blue), and F_Y = +0.015 au (green) conditions.