Supporting Information for

Mono- and bi-molecular adsorption of SF_6 decomposition products on Pt doped graphene: A First-principles investigation

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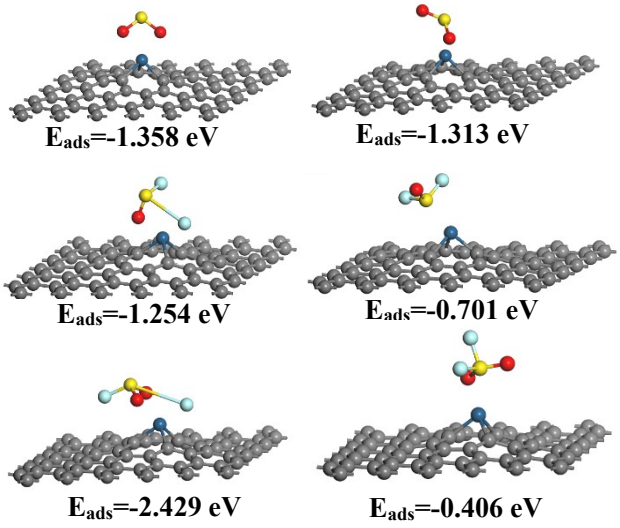

Figure. S1 Adsorption structure and adsorption energy comparison of single molecule adsorbed on Pt-graphene

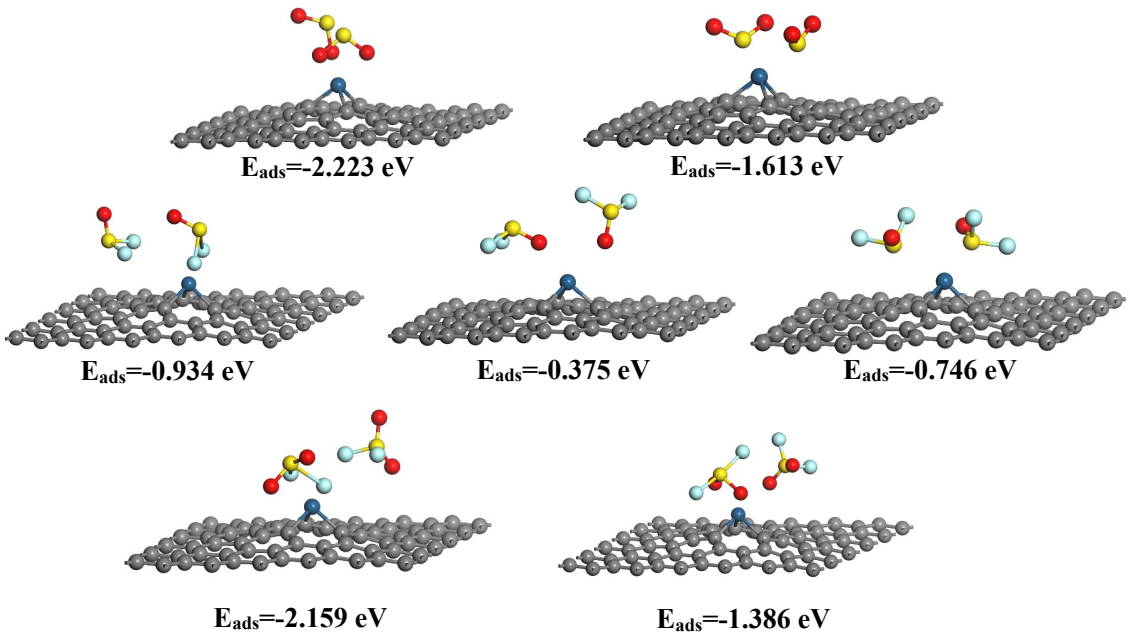

Figure. S2 Adsorption structure and adsorption energy comparison of double SO_2,SOF_2 and SO_2F_2 adsorbed on Pt-graphene

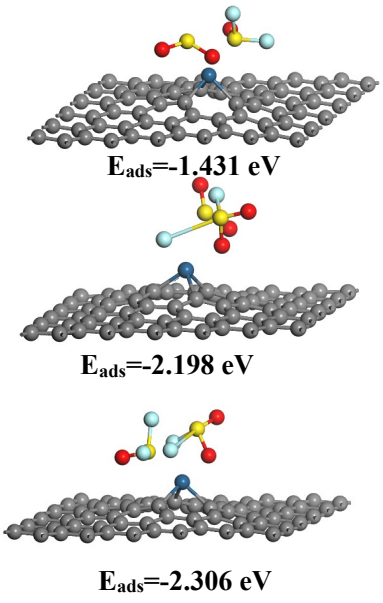

Figure. S3 Adsorption structure and adsorption energy comparison of double double foreign molecules adsorbed on Pt-graphene

Table S1. Cartesian coordinates of SO_2, SOF_2 and SO_2F_2

SO_2:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	S	-0.018310	0.089576	0.001678
2	O	1.459124	0.010603	0.000199
3	O	-0.685692	1.409671	0.026406

SOF_2:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	S	0.093980	-0.014937	0.047478
2	O	1.536188	0.040012	-0.170849
3	F	-0.479324	1.547479	-0.073436
4	F	-0.150844	-0.072554	1.696807

SO_2F_2:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	S	0.231329	-0.040518	-0.111754
2	O	1.652104	0.169111	-0.229558
3	F	-0.448301	1.379548	0.226512
4	F	-0.055036	-0.664453	1.345035

5	O	-0.618209	-0.721016	-1.056228

Table S2. Cartesian coordinates of graphene and Pt-graphene

Graphene:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	-0.182800	-0.682891	1.700015
2	C	-0.182808	0.737406	1.700036
3	C	2.277203	-0.682889	1.700196
4	C	2.277199	0.737419	1.700286
5	C	4.737202	-0.682892	1.700184
6	C	4.737211	0.737405	1.700286
7	C	7.197194	-0.682899	1.699989

8	C	7.197198	0.737411	1.700033
9	C	9.657199	-0.682918	1.699800
10	C	9.657189	0.737401	1.699818
11	C	12.117213	-0.682907	1.699814
12	C	12.117195	0.737383	1.699821
13	C	-1.412815	1.447512	1.699921
14	C	-1.412846	2.867816	1.699958
15	C	1.047192	1.447529	1.700203
16	C	1.047161	2.867822	1.700243
17	C	3.507203	1.447535	1.700407
18	C	3.507175	2.867819	1.700524
19	C	5.967192	1.447530	1.700213
20	C	5.967186	2.867858	1.700273
21	C	8.427197	1.447532	1.699927
22	C	8.427184	2.867836	1.699984
23	C	10.887178	1.447511	1.699815
24	C	10.887160	2.867812	1.699858
25	C	-2.642836	3.577933	1.699898
26	C	-2.642833	4.998229	1.699924
27	C	-0.182852	3.577937	1.700113
28	C	-0.182872	4.998209	1.700137
29	C	2.277146	3.577921	1.700464
30	C	2.277095	4.998156	1.700709
31	C	4.737158	3.577982	1.700489
32	C	4.737248	4.998252	1.700749
33	C	7.197175	3.577972	1.700156
34	C	7.197177	4.998282	1.700200
35	C	9.657172	3.577946	1.699917

36	C	9.657177	4.998270	1.699952
37	C	-3.872819	5.708375	1.699930
38	C	-3.872810	7.128678	1.699991
39	C	-1.412832	5.708340	1.699995
40	C	-1.412827	7.128654	1.699990
41	C	1.047167	5.708343	1.700313
42	C	1.047070	7.128631	1.700358
43	C	3.507224	5.708620	1.700954
44	C	3.506910	7.128463	1.703078
45	C	5.967143	5.708309	1.700379
46	C	5.967062	7.128773	1.700431
47	C	8.427198	5.708396	1.700052
48	C	8.427202	7.128703	1.700053
49	C	-5.102801	7.838800	1.700045
50	C	-5.102801	9.259114	1.700102
51	C	-2.642805	7.838791	1.700010
52	C	-2.642793	9.259097	1.700072
53	C	-0.182848	7.838763	1.700040
54	C	-0.182821	9.259084	1.700028
55	C	2.277368	7.838699	1.700417
56	C	2.277213	9.259124	1.700135
57	C	4.737533	7.839025	1.700459
58	C	4.737193	9.258955	1.700170
59	C	7.197211	7.838827	1.700118
60	C	7.197194	9.259101	1.700094
61	C	-6.332779	9.969236	1.700120
62	C	-6.332791	11.389522	1.700114
63	C	-3.872797	9.969223	1.700112

64	C	-3.872805	11.389522	1.700183
65	C	-1.412794	9.969219	1.700073
66	C	-1.412801	11.389535	1.700084
67	C	1.047203	9.969167	1.699913
68	C	1.047210	11.389498	1.699854
69	C	3.507107	9.969209	1.699911
70	C	3.507202	11.389491	1.699809
71	C	5.967222	9.969216	1.699967
72	C	5.967218	11.389516	1.699889

Pt-graphene:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	-0.182097	-0.680834	1.562051
2	C	-0.184259	0.738020	1.545513
3	C	2.277016	-0.683147	1.491546
4	C	2.276827	0.736514	1.523730
5	C	4.736955	-0.683147	1.491544
6	C	4.737145	0.736515	1.523727
7	C	7.196069	-0.680834	1.562046
8	C	7.198230	0.738020	1.545509
9	C	9.656754	-0.679490	1.671545
10	C	9.658308	0.737754	1.591755
11	C	12.117217	-0.679490	1.671547
12	C	12.115665	0.737755	1.591756
13	C	-1.413528	1.447553	1.562979

14	C	-1.413832	2.868338	1.581500
15	C	1.046231	1.444929	1.554493
16	C	1.041551	2.861721	1.643579
17	C	3.506986	1.444382	1.562867
18	C	3.506986	2.859532	1.698701
19	C	5.967741	1.444929	1.554490
20	C	5.972421	2.861721	1.643574
21	C	8.427499	1.447553	1.562976
22	C	8.427805	2.868339	1.581495
23	C	10.886986	1.448791	1.577121
24	C	10.886986	2.867889	1.555611
25	C	-2.643965	3.577293	1.568217
26	C	-2.642491	4.997008	1.575662
27	C	-0.185627	3.575306	1.654595
28	C	-0.183732	4.997556	1.747329
29	C	2.270440	3.559517	1.763685
30	C	2.259285	4.963434	2.008635
31	C	4.743531	3.559517	1.763682
32	C	4.754688	4.963436	2.008625
33	C	7.199599	3.575306	1.654589
34	C	7.197704	4.997557	1.747322
35	C	9.657936	3.577293	1.568213
36	C	9.656463	4.997007	1.575659
37	C	-3.873014	5.708009	1.549120
38	C	-3.873014	7.127609	1.532692
39	C	-1.415979	5.707185	1.652595
40	C	-1.420760	7.126442	1.642407
41	C	1.028878	5.698315	1.951093

42	C	1.005898	7.130595	2.019013
43	C	3.506986	5.547726	2.281011
44	Pt	3.506986	7.116946	3.432938
45	C	5.985093	5.698316	1.951080
46	C	6.008073	7.130594	2.019005
47	C	8.429950	5.707185	1.652590
48	C	8.434733	7.126443	1.642406
49	C	-5.101128	7.839249	1.549262
50	C	-5.102732	9.259337	1.524840
51	C	-2.644901	7.839249	1.549263
52	C	-2.643295	9.259338	1.524838
53	C	-0.203485	7.842721	1.770463
54	C	-0.190686	9.263573	1.710572
55	C	2.131958	7.919792	2.306503
56	C	2.255191	9.292334	2.033115
57	C	4.882012	7.919791	2.306500
58	C	4.758782	9.292335	2.033117
59	C	7.217456	7.842721	1.770462
60	C	7.204658	9.263573	1.710576
61	C	-6.330990	9.971222	1.571705
62	C	-6.332937	11.390336	1.531403
63	C	-3.873014	9.969328	1.488810
64	C	-3.873014	11.389391	1.479363
65	C	-1.415039	9.971222	1.571701
66	C	-1.413090	11.390335	1.531400
67	C	1.033883	9.984541	1.783115
68	C	1.044897	11.397665	1.657621
69	C	3.506986	9.989451	1.972687

70	C	3.506986	11.390467	1.768121
71	C	5.980089	9.984541	1.783119
72	C	5.969076	11.397664	1.657624

Table S3. Cartesian coordinates of single molecule adsorbed on Pt-graphene

SO_2 adsorption:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	0.016679	0.020750	-0.152415
2	C	0.015940	1.440449	-0.142294
3	C	-1.213692	2.151787	-0.188201
4	C	-1.215203	3.571034	-0.146119
5	C	-2.444038	4.282279	-0.188806
6	C	-2.445582	5.702821	-0.147963
7	C	-3.674986	6.413575	-0.153414
8	C	-3.674428	7.832905	-0.123521
9	C	-4.906621	8.542712	-0.093724
10	C	-4.904568	9.963559	-0.095575
11	C	-6.135884	10.672367	-0.093361
12	C	-6.134240	12.094259	-0.116152
13	C	2.476572	0.023566	-0.073357
14	C	2.475615	1.441835	0.003891
15	C	1.243839	2.146353	-0.033867
16	C	1.234209	3.561054	0.081568
17	C	0.010119	4.279048	-0.002835
18	C	-0.000629	5.698290	0.069023
19	C	-1.220268	6.414056	-0.047031
20	C	-1.214698	7.832998	-0.016820
21	C	-2.442319	8.543124	-0.088979
22	C	-2.444391	9.963922	-0.088107
23	C	-3.674497	10.673659	-0.100198

24	C	-3.674177	12.093989	-0.077508
25	C	4.935172	0.023159	-0.064046
26	C	4.937295	1.441286	0.015460
27	C	3.706724	2.157136	0.115933
28	C	3.708469	3.555552	0.336517
29	C	2.450416	4.255528	0.358995
30	C	2.332352	5.623433	0.627893
31	C	1.208351	6.405284	0.342387
32	C	1.231968	7.844514	0.307147
33	C	0.020542	8.541988	0.087715
34	C	0.015872	9.965974	-0.011280
35	C	-1.213394	10.673002	-0.079126
36	C	-1.214301	12.094440	-0.101234
37	C	7.394600	0.021380	-0.135265
38	C	7.395745	1.440807	-0.123008
39	C	6.168390	2.146888	-0.013359
40	C	6.177495	3.561464	0.109788
41	C	4.965231	4.258223	0.388324
42	C	5.067703	5.631037	0.679396
43	Pt	3.685039	6.421056	1.836291
44	C	3.706725	7.982537	0.644708
45	C	2.469033	8.581371	0.349951
46	C	2.472165	9.978553	0.070540
47	C	1.242710	10.678699	-0.042059
48	C	1.244944	12.095678	-0.141421
49	C	9.855413	0.021942	-0.189957
50	C	9.855153	1.442082	-0.224390
51	C	8.625241	2.151765	-0.171126

52	C	8.626402	3.571015	-0.128271
53	C	7.402382	4.278504	0.022187
54	C	7.409563	5.698087	0.085111
55	C	6.199532	6.402724	0.357370
56	C	6.179886	7.841553	0.297998
57	C	4.942455	8.577269	0.335893
58	C	4.938266	9.976680	0.058873
59	C	3.705663	10.680634	-0.011618
60	C	3.705540	12.095662	-0.155721
61	C	12.315642	0.021705	-0.198558
62	C	12.315922	1.442058	-0.233690
63	C	11.085579	2.152134	-0.244410
64	C	11.085418	3.572421	-0.227771
65	C	9.855067	4.282210	-0.180475
66	C	9.855605	5.702509	-0.142984
67	C	8.629657	6.413109	-0.041952
68	C	8.625832	7.831938	-0.022118
69	C	7.389842	8.540229	0.074996
70	C	7.394712	9.964804	-0.028453
71	C	6.167667	10.677289	-0.057324
72	C	6.165919	12.094833	-0.155575
73	O	3.624069	4.998433	3.595672
74	S	2.589250	5.849839	4.435154
75	O	2.393904	7.143466	3.546234

SOF_2 adsorption:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	0.013014	0.205481	-0.005436
2	C	0.011512	1.624608	0.007571
3	C	-1.217602	2.337398	-0.029440
4	C	-1.218162	3.756640	0.028671
5	C	-2.447922	4.467217	-0.004584
6	C	-2.446944	5.886854	0.047021
7	C	-3.678216	6.596834	0.042028
8	C	-3.677576	8.015674	0.068851
9	C	-4.910825	8.725082	0.092242
10	C	-4.908713	10.145524	0.078138
11	C	-6.140427	10.854730	0.070220
12	C	-6.139045	12.276265	0.034725
13	C	2.471820	0.204057	0.071198
14	C	2.469485	1.622151	0.142085
15	C	1.239038	2.329015	0.114165
16	C	1.231169	3.742401	0.243127
17	C	0.007615	4.462025	0.175551
18	C	0.006086	5.881416	0.261138
19	C	-1.217913	6.595622	0.147546
20	C	-1.214272	8.014135	0.169439
21	C	-2.443844	8.724343	0.096206
22	C	-2.446474	10.144864	0.082484
23	C	-3.677589	10.854624	0.064428
24	C	-3.678193	12.274954	0.071607

25	C	4.931641	0.203989	0.076627
26	C	4.932227	1.622232	0.147716
27	C	3.700413	2.335804	0.247382
28	C	3.697517	3.731476	0.472536
29	C	2.443966	4.434571	0.518628
30	C	2.367019	5.802052	0.824614
31	C	1.222584	6.580429	0.529809
32	C	1.237417	8.023406	0.483242
33	C	0.023361	8.721648	0.261103
34	C	0.015769	10.146769	0.148118
35	C	-1.214570	10.853532	0.078833
36	C	-1.217201	12.275618	0.044039
37	C	7.390166	0.205219	0.005747
38	C	7.390429	1.625104	0.017770
39	C	6.162144	2.329878	0.122599
40	C	6.169230	3.744387	0.247391
41	C	4.950884	4.435509	0.517472
42	C	5.048732	5.802692	0.809439
43	Pt	3.720909	6.623647	2.006379
44	C	3.707819	8.188046	0.823790
45	C	2.469887	8.773287	0.516340
46	C	2.470153	10.167211	0.219894
47	C	1.240162	10.864144	0.105702
48	C	1.240841	12.280935	0.000729
49	C	9.850585	0.209056	-0.047088
50	C	9.850030	1.629126	-0.074737
51	C	8.619245	2.337970	-0.021631
52	C	8.619467	3.757301	0.032408

53	C	7.392914	4.463711	0.176736
54	C	7.397528	5.883488	0.255909
55	C	6.183461	6.589178	0.520485
56	C	6.169094	8.029779	0.474124
57	C	4.938411	8.778903	0.509549
58	C	4.935526	10.169915	0.211925
59	C	3.701875	10.870652	0.134836
60	C	3.701270	12.283992	-0.012383
61	C	12.311833	0.209103	-0.053181
62	C	12.311671	1.629013	-0.079923
63	C	11.080712	2.338782	-0.084538
64	C	11.080684	3.758626	-0.052709
65	C	9.849418	4.467661	-0.003631
66	C	9.849999	5.887433	0.044994
67	C	8.621740	6.597473	0.143003
68	C	8.619411	8.015855	0.163188
69	C	7.383158	8.724889	0.252180
70	C	7.389354	10.149011	0.137855
71	C	6.164773	10.866060	0.094907
72	C	6.162552	12.281962	-0.009737
73	F	2.020413	5.294307	5.395432
74	S	3.640890	5.065002	4.980166
75	O	3.672513	4.878060	3.441331
76	F	4.326768	7.622510	3.643909

SO_2F_2 adsorption:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	-0.048504	-0.163795	0.223608
2	C	-0.049429	1.255336	0.236060
3	C	-1.278522	1.967608	0.191927
4	C	-1.279163	3.387215	0.242653
5	C	-2.508768	4.098023	0.200720
6	C	-2.509228	5.518037	0.246035
7	C	-3.739458	6.228324	0.240324
8	C	-3.739477	7.647300	0.269820
9	C	-4.973167	8.356369	0.298552
10	C	-4.970846	9.777287	0.292135
11	C	-6.202550	10.486117	0.290106
12	C	-6.200194	11.908164	0.262415
13	C	2.410555	-0.162602	0.301588
14	C	2.409206	1.256275	0.376285
15	C	1.177720	1.960781	0.344710
16	C	1.169476	3.374580	0.468245
17	C	-0.054805	4.093465	0.391052
18	C	-0.060755	5.513215	0.467592
19	C	-1.281983	6.227533	0.347103
20	C	-1.276112	7.646282	0.369916
21	C	-2.505827	8.356380	0.298768
22	C	-2.508182	9.777305	0.292101
23	C	-3.739494	10.487245	0.281091
24	C	-3.739528	11.908066	0.296463
25	C	4.870427	-0.162589	0.301127

26	C	4.871733	1.256321	0.375648
27	C	3.640531	1.971855	0.480787
28	C	3.640489	3.368070	0.714662
29	C	2.380436	4.066511	0.753138
30	C	2.279377	5.432345	1.057107
31	C	1.149882	6.214422	0.746846
32	C	1.175717	7.658248	0.694802
33	C	-0.038567	8.354038	0.463541
34	C	-0.045661	9.778908	0.353995
35	C	-1.276420	10.486128	0.289809
36	C	-1.278875	11.908214	0.261775
37	C	7.329449	-0.163697	0.222669
38	C	7.330331	1.255422	0.234807
39	C	6.103205	1.960891	0.343457
40	C	6.111273	3.374768	0.466684
41	C	4.900520	4.066765	0.751867
42	C	5.001627	5.432947	1.055478
43	Pt	3.641098	6.224591	2.216247
44	C	3.640222	7.811364	1.058277
45	C	2.408752	8.406485	0.726958
46	C	2.407958	9.796740	0.428053
47	C	1.179171	10.495139	0.314048
48	C	1.179766	11.911873	0.214311
49	C	9.789878	-0.161069	0.167628
50	C	9.789844	1.258694	0.138664
51	C	8.559508	1.967664	0.190758
52	C	8.560110	3.387236	0.241343
53	C	7.335748	4.093553	0.389341

54	C	7.341838	5.513153	0.466031
55	C	6.131173	6.214375	0.745276
56	C	6.105275	7.658087	0.694191
57	C	4.872299	8.406410	0.727116
58	C	4.873007	9.796571	0.428242
59	C	3.640450	10.500261	0.348777
60	C	3.640488	11.912465	0.204625
61	C	12.251096	-0.161098	0.168094
62	C	12.251124	1.258686	0.139280
63	C	11.020507	1.968735	0.128021
64	C	11.020499	3.388534	0.153718
65	C	9.789784	4.098042	0.199998
66	C	9.790308	5.518055	0.245377
67	C	8.563028	6.227543	0.346087
68	C	8.557119	7.646278	0.369343
69	C	7.319549	8.354084	0.463134
70	C	7.326610	9.778869	0.354164
71	C	6.101799	10.495058	0.314376
72	C	6.101159	11.911835	0.214966
73	O	2.423646	7.284663	3.857619
74	S	3.643133	7.892118	4.578900
75	F	3.640437	9.503002	3.956903
76	F	3.642221	4.638078	3.480588
77	O	4.863400	7.287016	3.856359

Table S4. Cartesian coordinates of double molecule ($2SO_2$, $2SOF_2$, $2SO_2F_2$) adsorbed on Pt-graphene

$2SO_2$:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	-0.021005	-0.035775	-0.225668
2	C	-0.022055	1.383636	-0.215412
3	C	-1.252063	2.094387	-0.264443
4	C	-1.253257	3.513625	-0.222510
5	C	-2.482350	4.225003	-0.267883
6	C	-2.483024	5.645449	-0.228407
7	C	-3.712071	6.356498	-0.233203
8	C	-3.711518	7.775914	-0.202152
9	C	-4.943710	8.485720	-0.169909
10	C	-4.942021	9.906935	-0.167574
11	C	-6.173304	10.615904	-0.165506
12	C	-6.171878	12.037943	-0.186193
13	C	2.438715	-0.032307	-0.139787
14	C	2.436814	1.386539	-0.062737
15	C	1.205001	2.090622	-0.103991
16	C	1.195718	3.505318	0.012916
17	C	-0.029294	4.221328	-0.075602
18	C	-0.037686	5.640468	-0.005710
19	C	-1.257265	6.355835	-0.127389
20	C	-1.251145	7.774559	-0.096844
21	C	-2.479005	8.485568	-0.167527
22	C	-2.481293	9.906710	-0.162204

23	C	-3.711546	10.617051	-0.169653
24	C	-3.711914	12.038007	-0.143478
25	C	4.897628	-0.032488	-0.130694
26	C	4.898697	1.386464	-0.051617
27	C	3.667564	2.103518	0.049427
28	C	3.666212	3.502556	0.272937
29	C	2.405433	4.202179	0.302759
30	C	2.299678	5.571516	0.595759
31	C	1.169018	6.341949	0.280042
32	C	1.194973	7.782523	0.235767
33	C	-0.015003	8.482397	0.008522
34	C	-0.020315	9.907355	-0.089883
35	C	-1.249914	10.615521	-0.153661
36	C	-1.251920	12.037645	-0.171851
37	C	7.356942	-0.035689	-0.207594
38	C	7.357527	1.384037	-0.194451
39	C	6.130337	2.091244	-0.083270
40	C	6.138822	3.506433	0.035504
41	C	4.926215	4.204532	0.315187
42	C	5.034657	5.577953	0.598288
43	Pt	3.665606	6.373375	1.763398
44	C	3.673099	7.929401	0.567729
45	C	2.432598	8.522011	0.273371
46	C	2.435709	9.919512	-0.010696
47	C	1.206108	10.620302	-0.121738
48	C	1.207343	12.037909	-0.218891
49	C	9.817457	-0.035588	-0.269217
50	C	9.817114	1.384640	-0.301867

51	C	8.587165	2.094691	-0.245837
52	C	8.588185	3.514016	-0.204519
53	C	7.364360	4.221979	-0.054919
54	C	7.373419	5.641596	0.005498
55	C	6.165976	6.346029	0.280238
56	C	6.142941	7.785371	0.224884
57	C	4.906625	8.523578	0.259601
58	C	4.901397	9.920306	-0.022923
59	C	3.668015	10.622703	-0.094569
60	C	3.667729	12.037746	-0.237345
61	C	12.277687	-0.035712	-0.278850
62	C	12.277862	1.384517	-0.312381
63	C	11.047294	2.094747	-0.323008
64	C	11.047324	3.514983	-0.306502
65	C	9.817106	4.225164	-0.258555
66	C	9.818620	5.645604	-0.222047
67	C	8.593188	6.356230	-0.120859
68	C	8.588318	7.775103	-0.099246
69	C	7.352579	8.483580	-0.001395
70	C	7.357029	9.908222	-0.104138
71	C	6.130376	10.620878	-0.136923
72	C	6.128555	12.038156	-0.234017
73	O	3.458727	4.855924	3.523199
74	S	2.758577	5.914533	4.432566
75	O	2.210661	6.991697	3.438256
76	O	4.353580	8.685108	5.117947
77	S	4.896509	7.337038	4.755498
78	O	5.194665	7.136468	3.236644

$2SOF_2$:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	-0.100209	0.162890	-0.195322
2	C	-0.101936	1.582354	-0.185796
3	C	-1.332143	2.292277	-0.233593
4	C	-1.334151	3.711375	-0.190996
5	C	-2.562571	4.423065	-0.238704
6	C	-2.563557	5.843648	-0.198225
7	C	-3.791831	6.555075	-0.205025
8	C	-3.790473	7.974606	-0.171667
9	C	-5.021660	8.685061	-0.140645
10	C	-5.020169	10.106064	-0.138099
11	C	-6.251341	10.815402	-0.135083
12	C	-6.250709	12.237156	-0.156709
13	C	2.359645	0.167122	-0.112469
14	C	2.357323	1.585860	-0.037755
15	C	1.125206	2.289342	-0.076190
16	C	1.114438	3.703695	0.044436
17	C	-0.110629	4.418752	-0.041961
18	C	-0.121086	5.837742	0.028700
19	C	-1.338918	6.554400	-0.094030
20	C	-1.332245	7.973129	-0.061502
21	C	-2.558937	8.684703	-0.133268

22	C	-2.560568	10.105680	-0.129459
23	C	-3.790440	10.816419	-0.139920
24	C	-3.790840	12.237264	-0.116413
25	C	4.818400	0.166921	-0.103971
26	C	4.819433	1.586604	-0.031521
27	C	3.588065	2.303948	0.067248
28	C	3.588176	3.704402	0.282947
29	C	2.327141	4.399490	0.328015
30	C	2.209879	5.766218	0.625637
31	C	1.084046	6.540924	0.311413
32	C	1.112657	7.979257	0.259773
33	C	-0.096696	8.681009	0.042039
34	C	-0.100342	10.105612	-0.055437
35	C	-1.329458	10.814471	-0.119462
36	C	-1.331041	12.236614	-0.140832
37	C	7.277812	0.163370	-0.176881
38	C	7.277812	1.583925	-0.169585
39	C	6.050089	2.293293	-0.065070
40	C	6.056538	3.710459	0.046038
41	C	4.843707	4.413274	0.317939
42	C	4.939724	5.791556	0.605476
43	Pt	3.556346	6.580466	1.782568
44	C	3.597469	8.121572	0.561087
45	C	2.352047	8.712572	0.286476
46	C	2.357194	10.114793	0.018529
47	C	1.126822	10.817236	-0.086388
48	C	1.128244	12.235526	-0.184228
49	C	9.738350	0.162059	-0.235454

50	C	9.737445	1.582742	-0.272358
51	C	8.507654	2.293666	-0.221830
52	C	8.508141	3.713163	-0.184642
53	C	7.284004	4.422189	-0.040505
54	C	7.293829	5.841283	0.024189
55	C	6.085411	6.544416	0.293783
56	C	6.069098	7.982050	0.240472
57	C	4.832911	8.716671	0.276716
58	C	4.823470	10.117959	0.009221
59	C	3.589613	10.819029	-0.061356
60	C	3.588452	12.235312	-0.201979
61	C	12.198247	0.161971	-0.244512
62	C	12.197881	1.582413	-0.280358
63	C	10.967609	2.292659	-0.293976
64	C	10.967259	3.713255	-0.279634
65	C	9.737308	4.423687	-0.235728
66	C	9.739254	5.844202	-0.197732
67	C	8.514361	6.555301	-0.097814
68	C	8.511443	7.973928	-0.073351
69	C	7.276803	8.682925	0.024196
70	C	7.279894	10.107499	-0.073548
71	C	6.052608	10.819191	-0.102725
72	C	6.049369	12.236451	-0.200315
73	F	2.444817	6.867491	3.429811
74	S	4.893038	7.570737	5.065990
75	O	5.243253	6.242305	5.676092
76	F	5.208538	7.468928	3.296243
77	F	5.710020	3.694491	3.486313

78	S	4.735553	2.392556	3.868112
79	O	4.884588	2.138615	5.297982
80	F	3.329699	3.280227	3.664053

$2SO_2F_2$:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	0.011181	-0.081249	-0.265811
2	C	0.008055	1.337013	-0.250894
3	C	-1.221727	2.048567	-0.290279
4	C	-1.223660	3.467930	-0.237534
5	C	-2.452552	4.179618	-0.279970
6	C	-2.451399	5.599700	-0.234649
7	C	-3.680270	6.310835	-0.247432
8	C	-3.677626	7.729978	-0.217145
9	C	-4.910151	8.439945	-0.198444
10	C	-4.908430	9.860875	-0.200510
11	C	-6.139791	10.570790	-0.206693
12	C	-6.139273	11.992111	-0.229336
13	C	2.471134	-0.079107	-0.184332
14	C	2.467622	1.339496	-0.107850
15	C	1.234661	2.041970	-0.141086
16	C	1.223423	3.453940	-0.009957
17	C	-0.000573	4.173004	-0.084937
18	C	-0.005223	5.592216	-0.002975
19	C	-1.224383	6.308334	-0.126603

20	C	-1.215621	7.727188	-0.097701
21	C	-2.444277	8.438646	-0.175090
22	C	-2.446563	9.859628	-0.177161
23	C	-3.677526	10.570445	-0.198522
24	C	-3.678780	11.991481	-0.180876
25	C	4.930573	-0.079122	-0.166124
26	C	4.929931	1.340768	-0.097008
27	C	3.697864	2.055907	0.000022
28	C	3.693107	3.454412	0.227880
29	C	2.429930	4.146287	0.281622
30	C	2.337452	5.510091	0.603700
31	C	1.204829	6.288679	0.284653
32	C	1.235825	7.731855	0.232019
33	C	0.022608	8.433321	0.004403
34	C	0.015430	9.858917	-0.097192
35	C	-1.214875	10.567961	-0.166315
36	C	-1.218493	11.990577	-0.193988
37	C	7.389169	-0.081036	-0.228883
38	C	7.388316	1.339438	-0.225677
39	C	6.160091	2.047370	-0.125918
40	C	6.166856	3.463855	-0.017383
41	C	4.949982	4.158361	0.255796
42	C	5.068616	5.531714	0.533507
43	Pt	3.731909	6.300414	1.728594
44	C	3.720583	7.875241	0.550407
45	C	2.475271	8.474648	0.261653
46	C	2.470912	9.872998	-0.022370
47	C	1.240751	10.574098	-0.130360

48	C	1.239573	11.992305	-0.232617
49	C	9.848467	-0.079494	-0.286567
50	C	9.847103	1.340890	-0.323682
51	C	8.616977	2.051190	-0.274920
52	C	8.616520	3.471095	-0.240012
53	C	7.391865	4.179761	-0.104021
54	C	7.401887	5.598578	-0.045938
55	C	6.195601	6.307644	0.223444
56	C	6.174579	7.745313	0.179512
57	C	4.942008	8.487767	0.228223
58	C	4.936540	9.880121	-0.052661
59	C	3.701142	10.580068	-0.113703
60	C	3.698965	11.993978	-0.257488
61	C	12.309162	-0.079631	-0.305720
62	C	12.307884	1.340240	-0.337055
63	C	11.077304	2.050529	-0.344102
64	C	11.076789	3.470735	-0.325693
65	C	9.846571	4.181048	-0.285203
66	C	9.849347	5.601089	-0.249133
67	C	8.623129	6.311951	-0.160085
68	C	8.620643	7.730251	-0.137694
69	C	7.386075	8.440410	-0.046097
70	C	7.390151	9.864359	-0.145624
71	C	6.164244	10.578983	-0.173958
72	C	6.160856	11.994924	-0.268765
73	O	7.334464	7.056593	4.806178
74	S	6.497921	5.946394	4.281763
75	F	3.414572	5.017987	3.242629

76	F	5.010385	7.272937	3.050613
77	O	7.055163	5.150943	3.148518
78	O	0.747152	8.691665	5.953368
79	S	1.094263	8.719654	4.554875
80	F	2.607176	9.243030	4.423995
81	F	1.437127	7.214445	4.097544
82	O	0.326195	9.330667	3.494377

Table S5. Cartesian coordinates of double molecule (SO_2& SOF_2, SO_2& SO_2F_2, SOF_2& SO_2F_2) adsorbed on Pt-graphene

SO_2& SOF_2:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	0.005674	-0.059858	-0.158059
2	C	0.004322	1.359875	-0.141282
3	C	-1.225705	2.070240	-0.182086
4	C	-1.226940	3.489659	-0.124260
5	C	-2.456504	4.200545	-0.166411
6	C	-2.456669	5.620421	-0.117658
7	C	-3.686278	6.331074	-0.127242
8	C	-3.685568	7.750329	-0.097755
9	C	-4.917559	8.460222	-0.075160

10	C	-4.915633	9.881159	-0.083359
11	C	-6.147145	10.590243	-0.090559
12	C	-6.145822	12.012138	-0.118516
13	C	2.464670	-0.058782	-0.076483
14	C	2.462605	1.359867	0.000372
15	C	1.231922	2.066004	-0.029241
16	C	1.223362	3.479997	0.104656
17	C	-0.003563	4.195473	0.031340
18	C	-0.010191	5.614819	0.111767
19	C	-1.230335	6.330181	-0.011012
20	C	-1.225897	7.749094	0.014797
21	C	-2.453537	8.460064	-0.063358
22	C	-2.455260	9.880690	-0.073799
23	C	-3.685574	10.591093	-0.090968
24	C	-3.685842	12.011850	-0.078459
25	C	4.923419	-0.058472	-0.072072
26	C	4.924053	1.360600	-0.000028
27	C	3.692861	2.075889	0.106789
28	C	3.691225	3.473376	0.336214
29	C	2.435015	4.173549	0.395474
30	C	2.328091	5.536331	0.736378
31	C	1.199332	6.313429	0.398089
32	C	1.222851	7.755262	0.330190
33	C	0.010586	8.456206	0.107072
34	C	0.005954	9.880542	-0.011813
35	C	-1.223592	10.589147	-0.076549
36	C	-1.225802	12.011674	-0.108533
37	C	7.382094	-0.059982	-0.148316

38	C	7.382124	1.360328	-0.138022
39	C	6.154125	2.067582	-0.031735
40	C	6.161480	3.482824	0.088080
41	C	4.946432	4.178207	0.368619
42	C	5.056631	5.545312	0.667564
43	Pt	3.722448	6.346937	1.899525
44	C	3.699001	7.904828	0.604914
45	C	2.462650	8.496529	0.323459
46	C	2.462047	9.894831	0.037033
47	C	1.231830	10.595658	-0.060060
48	C	1.232601	12.013453	-0.158906
49	C	9.843041	-0.059517	-0.209738
50	C	9.842294	1.361237	-0.235827
51	C	8.611786	2.071067	-0.182275
52	C	8.612228	3.490438	-0.133161
53	C	7.387339	4.197762	0.011557
54	C	7.395679	5.616870	0.083706
55	C	6.187105	6.321041	0.358323
56	C	6.168569	7.760101	0.300281
57	C	4.932432	8.500686	0.320042
58	C	4.928635	9.897211	0.034202
59	C	3.694477	10.598089	-0.044723
60	C	3.693599	12.014423	-0.180171
61	C	12.304056	-0.059316	-0.213910
62	C	12.303903	1.361108	-0.237490
63	C	11.072957	2.070906	-0.246237
64	C	11.072828	3.491317	-0.217517
65	C	9.842136	4.200733	-0.172747

66	C	9.843749	5.620856	-0.127651
67	C	8.617340	6.331428	-0.031788
68	C	8.614631	7.749816	-0.007560
69	C	7.378654	8.458382	0.081513
70	C	7.383473	9.882807	-0.029396
71	C	6.157833	10.597386	-0.072009
72	C	6.155298	12.014617	-0.168704
73	O	5.332856	6.936195	3.349235
74	S	5.078228	5.469423	3.905536
75	O	6.146020	4.465743	3.582070
76	F	2.702643	7.133029	5.033988
77	S	2.022197	7.121433	3.538871
78	O	0.725813	6.470002	3.649801
79	F	1.765403	8.762039	3.572966

SO_2& SO_2F_2:

Final Coordinates (Angstroms)

ATOM		X	Y	Z
1	C	-0.169137	0.104140	-0.249925
2	C	-0.169294	1.523919	-0.245198
3	C	-1.397949	2.236810	-0.284176
4	C	-1.398274	3.656460	-0.235930
5	C	-2.628061	4.366890	-0.273815
6	C	-2.629097	5.786739	-0.225814
7	C	-3.860481	6.496067	-0.231409
8	C	-3.861200	7.914991	-0.200581

9	C	-5.095178	8.623466	-0.172028
10	C	-5.092550	10.044304	-0.179653
11	C	-6.324393	10.753147	-0.178856
12	C	-6.321479	12.175204	-0.214070
13	C	2.289652	0.103836	-0.188364
14	C	2.289526	1.522655	-0.126273
15	C	1.059296	2.229180	-0.150284
16	C	1.052234	3.644083	-0.031333
17	C	-0.171961	4.363307	-0.096773
18	C	-0.177994	5.782759	-0.015926
19	C	-1.401440	6.496846	-0.125792
20	C	-1.397887	7.915285	-0.100567
21	C	-2.627912	8.624522	-0.171176
22	C	-2.629852	10.045146	-0.181858
23	C	-3.861218	10.754343	-0.196436
24	C	-3.860414	12.174935	-0.191972
25	C	4.749890	0.103806	-0.195677
26	C	4.752565	1.522277	-0.134969
27	C	3.521614	2.236623	-0.035548
28	C	3.525785	3.633040	0.185986
29	C	2.270481	4.334524	0.234913
30	C	2.166674	5.700590	0.533240
31	C	1.034789	6.488841	0.252325
32	C	1.052348	7.929968	0.220417
33	C	-0.161970	8.624657	-0.004998
34	C	-0.167815	10.048877	-0.113924
35	C	-1.398169	10.754565	-0.185976
36	C	-1.399337	12.175816	-0.225374

37	C	7.209101	0.104175	-0.265817
38	C	7.211138	1.522769	-0.263470
39	C	5.983701	2.227397	-0.166243
40	C	5.992515	3.640672	-0.047013
41	C	4.781983	4.332019	0.227528
42	C	4.861355	5.697068	0.540907
43	Pt	3.501078	6.491507	1.729375
44	C	3.512169	8.079988	0.587671
45	C	2.283286	8.678962	0.268761
46	C	2.285550	10.069532	-0.026593
47	C	1.056995	10.765629	-0.150112
48	C	1.059354	12.180991	-0.260104
49	C	9.669921	0.107947	-0.303529
50	C	9.670355	1.527777	-0.341095
51	C	8.439887	2.236018	-0.301523
52	C	8.440258	3.655617	-0.252200
53	C	7.215273	4.360817	-0.113513
54	C	7.216713	5.779532	-0.030075
55	C	6.002147	6.476540	0.245289
56	C	5.982712	7.920353	0.216792
57	C	4.749522	8.670516	0.268704
58	C	4.750646	10.065292	-0.022221
59	C	3.519302	10.770418	-0.103244
60	C	3.520238	12.182664	-0.255628
61	C	12.130849	0.107966	-0.295383
62	C	12.131385	1.527939	-0.331180
63	C	10.901081	2.237653	-0.347378
64	C	10.900974	3.657568	-0.323252

65	C	9.669936	4.366190	-0.282787
66	C	9.668985	5.785791	-0.232734
67	C	8.439817	6.493999	-0.135887
68	C	8.434869	7.912618	-0.104879
69	C	7.197120	8.620100	-0.005996
70	C	7.204995	10.045998	-0.107917
71	C	5.980328	10.762889	-0.141628
72	C	5.980213	12.179850	-0.247800
73	O	7.398058	6.645431	5.330211
74	S	6.696337	6.236144	4.093509
75	O	7.257288	5.122702	3.285343
76	O	2.858814	3.324963	4.875981
77	S	3.028371	4.740647	4.468186
78	F	2.709926	7.459713	3.304129
79	F	4.474505	5.249009	5.338949
80	O	3.652583	4.757468	3.009815

SOF_2& SO_2F_2:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	-0.110979	0.050999	-0.169912
2	C	-0.109706	1.472170	-0.167241
3	C	-1.339235	2.181515	-0.219612
4	C	-1.339257	3.601320	-0.194455
5	C	-2.568662	4.311450	-0.249136
6	C	-2.572371	5.731971	-0.221401

7	C	-3.800917	6.442557	-0.227498
8	C	-3.803964	7.862131	-0.195502
9	C	-5.035821	8.571747	-0.151296
10	C	-5.034158	9.993103	-0.141955
11	C	-6.265473	10.701734	-0.122991
12	C	-6.262397	12.124535	-0.140874
13	C	2.348266	0.056040	-0.114499
14	C	2.349057	1.476656	-0.048267
15	C	1.118808	2.183047	-0.074281
16	C	1.113461	3.601607	0.022907
17	C	-0.114948	4.311730	-0.064705
18	C	-0.127694	5.730377	-0.020022
19	C	-1.348175	6.443898	-0.134102
20	C	-1.345680	7.862442	-0.113976
21	C	-2.573136	8.573106	-0.172052
22	C	-2.574079	9.994403	-0.166381
23	C	-3.804051	10.704804	-0.158467
24	C	-3.802735	12.126236	-0.134062
25	C	4.807226	0.055904	-0.138685
26	C	4.811081	1.474960	-0.067415
27	C	3.581206	2.193815	0.039715
28	C	3.586341	3.595866	0.252567
29	C	2.330470	4.305872	0.278377
30	C	2.218445	5.687641	0.542217
31	C	1.077950	6.439079	0.234091
32	C	1.095403	7.873952	0.189944
33	C	-0.112324	8.573168	-0.023422
34	C	-0.114046	9.997069	-0.111599

35	C	-1.342955	10.704611	-0.167767
36	C	-1.342753	12.125950	-0.185236
37	C	7.267722	0.050559	-0.221101
38	C	7.271201	1.468894	-0.213549
39	C	6.044627	2.175846	-0.110413
40	C	6.057230	3.588813	0.005493
41	C	4.851737	4.285378	0.297906
42	C	4.956325	5.649188	0.617728
43	Pt	3.569762	6.448047	1.754373
44	C	3.554014	7.995978	0.536750
45	C	2.330564	8.607266	0.236994
46	C	2.341426	10.006957	-0.019282
47	C	1.113516	10.708461	-0.133098
48	C	1.117855	12.125012	-0.221098
49	C	9.729992	0.049397	-0.254841
50	C	9.731449	1.469472	-0.291430
51	C	8.501629	2.178525	-0.255944
52	C	8.504259	3.597586	-0.218136
53	C	7.281738	4.303730	-0.078091
54	C	7.290353	5.722245	-0.003928
55	C	6.085068	6.418981	0.289125
56	C	6.049634	7.859257	0.243065
57	C	4.806153	8.591198	0.272308
58	C	4.806416	9.997390	0.013947
59	C	3.576675	10.705826	-0.071606
60	C	3.579480	12.122421	-0.204661
61	C	12.189523	0.049569	-0.228633
62	C	12.191165	1.470228	-0.267835

63	C	10.961595	2.179849	-0.297917
64	C	10.962195	3.600332	-0.290688
65	C	9.732419	4.309735	-0.259098
66	C	9.732522	5.730206	-0.221269
67	C	8.507441	6.440009	-0.120091
68	C	8.497376	7.858874	-0.080758
69	C	7.259888	8.565139	0.026808
70	C	7.264867	9.991178	-0.059055
71	C	6.037354	10.702310	-0.083924
72	C	6.038518	12.122119	-0.175319
73	O	2.070595	7.368731	3.008398
74	S	1.526721	6.547117	4.250299
75	F	0.928793	5.143160	3.365657
76	F	4.532307	6.026256	3.492824
77	O	0.309599	7.225629	4.755096
78	F	8.781402	5.793365	3.865274
79	S	7.117607	5.559555	3.701018
80	O	6.970639	4.163685	3.280872
81	F	6.868390	5.601406	5.343977
