

Supporting materials

Yong Han^{a,b*}, Huiqing Yang^b, Qingrui Zhang^c, Tifeng Jiao^{a*}

a State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao Hebei 066004, P. R. China.

b School of Electrical Engineering, Yanshan University, Qinhuangdao Hebei 066004, P. R. China.

c School of Environmental and Chemical Engineering, Yanshan University, Qinhuangdao Hebei 066004, P. R. China.

Corresponding Author

* Yong Han E-mail addresses: hanyong@ysu.edu.cn

* Tifeng Jiao E-mail addresses: tfjiao@ysu.edu.cn

This *Supplemental file* contains:

1. In Table S1, IRC transition state structures for the reaction of sulfate radical (SR) with phenol in the +X-axis electric field (calculated absolute energies).
2. In Table S2, IRC transition state structures for the reaction of sulfate radical (SR) with phenol in the -X-axis electric field (calculated absolute energies).
3. In Table S3, The atomic coordinate position without an external electric field.
- 4 In Table S4, Atomic coordinates under an externally applied negative electric field of 0.0002 a.u..
5. In Table S5, Atomic coordinates under an externally applied negative electric field of 0.0005 a.u..
6. In Table S6, Atomic coordinates under an externally applied negative electric field of 0.001 a.u..
7. In Table S7, Atomic coordinates under an externally applied negative electric field of 0.002 a.u..
8. In Table S8, Atomic coordinates under an externally applied positive electric field of 0.0002 a.u..
9. In Table S9, Atomic coordinates under an externally applied positive electric field

of 0.0005 a.u..

10. In Table S10, Atomic coordinates under an externally applied positive electric field of 0.001 a.u..

11. In Table S11, Atomic coordinates under an externally applied positive electric field of 0.002 a.u..

Table S1 IRC transition state structures for the reaction of sulfate radical (SR) with phenol in the +X-axis electric field (calculated absolved energies)

	Total Energy (Hartree)				
(step))EF strength(a.u.)	0	0.0002	0.0005	0.001	0.002
1	-1006.3587	-1006.35771	-1006.35612	-1006.35352	-1006.3513
2	-1006.3587	-1006.35772	-1006.35613	-1006.3535	-1006.35127
3	-1006.3587	-1006.35772	-1006.35613	-1006.35347	-1006.35125
4	-1006.3587	-1006.35772	-1006.35613	-1006.35345	-1006.35122
5	-1006.3587	-1006.35772	-1006.35613	-1006.35342	-1006.3512
6	-1006.35869	-1006.35771	-1006.35612	-1006.3534	-1006.35117
7	-1006.35869	-1006.35771	-1006.35612	-1006.35337	-1006.35115
8	-1006.35869	-1006.35772	-1006.35613	-1006.35335	-1006.35112
9	-1006.35868	-1006.35771	-1006.35612	-1006.35332	-1006.3511
10	-1006.35868	-1006.35772	-1006.35613	-1006.3533	-1006.35107
11	-1006.35867	-1006.35772	-1006.35613	-1006.35327	-1006.35105
12	-1006.35866	-1006.35772	-1006.35613	-1006.35325	-1006.35102
13	-1006.35864	-1006.35772	-1006.35613	-1006.35322	-1006.351
14	-1006.35862	-1006.35772	-1006.35613	-1006.35319	-1006.35097
15	-1006.35858	-1006.35769	-1006.3561	-1006.35317	-1006.35095
16	-1006.35854	-1006.35766	-1006.35607	-1006.35314	-1006.35092
17	-1006.3585	-1006.35763	-1006.35604	-1006.35312	-1006.35089
18	-1006.35844	-1006.35758	-1006.35599	-1006.35309	-1006.35087
19	-1006.35839	-1006.35756	-1006.35597	-1006.35306	-1006.35084
20	-1006.35832	-1006.35749	-1006.3559	-1006.35304	-1006.35082
21	-1006.35824	-1006.35741	-1006.35582	-1006.35301	-1006.35079
22	-1006.35816	-1006.35731	-1006.35572	-1006.35299	-1006.35076
23	-1006.35806	-1006.35711	-1006.35552	-1006.35296	-1006.35074
24	-1006.35797	-1006.35692	-1006.35533	-1006.35293	-1006.35071
25	-1006.35788	-1006.35665	-1006.35506	-1006.35291	-1006.35069
26	-1006.35781	-1006.35636	-1006.35477	-1006.35288	-1006.35066
27	-1006.35778	-1006.35612	-1006.35453	-1006.35285	-1006.35063
28	-1006.35781	-1006.35599	-1006.3544	-1006.35282	-1006.35061
29	-1006.3579	-1006.35598	-1006.35439	-1006.3528	-1006.35058
30	-1006.35803	-1006.35605	-1006.35446	-1006.35277	-1006.35055
31	-1006.35819	-1006.35619	-1006.3546	-1006.35274	-1006.35052
32	-1006.35836	-1006.35637	-1006.35478	-1006.35271	-1006.3505
33	-1006.35853	-1006.35655	-1006.35496	-1006.35268	-1006.35047
34	-1006.3587	-1006.35673	-1006.35514	-1006.35265	-1006.35044
35	-1006.35886	-1006.35689	-1006.3553	-1006.35262	-1006.35041
36	-1006.35901	-1006.35702	-1006.35543	-1006.35259	-1006.35038
37	-1006.35916	-1006.35713	-1006.35554	-1006.35256	-1006.35035
38	-1006.35931	-1006.3572	-1006.35561	-1006.35253	-1006.35032

39	-1006.35948	-1006.35727	-1006.35568	-1006.35249	-1006.35029
40	-1006.35967	-1006.35732	-1006.35573	-1006.35245	-1006.35026
41	-1006.35988	-1006.35731	-1006.35572	-1006.35241	-1006.35023
42	-1006.36015	-1006.35732	-1006.35573	-1006.35238	-1006.35019
43	-1006.36048	-1006.35733	-1006.35574	-1006.35234	-1006.35015
44	-1006.36091	-1006.35741	-1006.35582	-1006.3523	-1006.35011
45	-1006.36144	-1006.35756	-1006.35597	-1006.35225	-1006.35008
46	-1006.36209	-1006.35783	-1006.35624	-1006.35222	-1006.35004
47	-1006.36287	-1006.35824	-1006.35665	-1006.35217	-1006.35
48	-1006.36378	-1006.35883	-1006.35724	-1006.35214	-1006.34995
49	-1006.36483	-1006.35962	-1006.35803	-1006.35211	-1006.34992
50	-1006.36598	-1006.3606	-1006.35901	-1006.35208	-1006.34987
51	-1006.36724	-1006.36183	-1006.36024	-1006.35203	-1006.34984
52	-1006.36856	-1006.36327	-1006.36168	-1006.35199	-1006.34981
53	-1006.36991	-1006.36493	-1006.36334	-1006.35194	-1006.34978
54	-1006.37123	-1006.36671	-1006.36512	-1006.35188	-1006.34973
55	-1006.37246	-1006.36851	-1006.36692	-1006.35185	-1006.34969
56	-1006.37355	-1006.3702	-1006.36861	-1006.3518	-1006.34964
57	-1006.37444	-1006.3716	-1006.37001	-1006.35173	-1006.34958
58	-1006.37513	-1006.37265	-1006.37106	-1006.35166	-1006.34955
59	-1006.37566	-1006.37351	-1006.37192	-1006.35158	-1006.3495
60	-1006.37606	-1006.37416	-1006.37257	-1006.35148	-1006.34943
61	-1006.37634	-1006.37452	-1006.37293	-1006.35138	-1006.34936
62	-1006.37662	-1006.37494	-1006.37335	-1006.35127	-1006.34928
63	-1006.37676	-1006.37512	-1006.37353	-1006.35115	-1006.34918
64	-1006.37691	-1006.37537	-1006.37378	-1006.35101	-1006.34908
65	-1006.37709	-1006.3756	-1006.37401	-1006.35087	-1006.34897
66	-1006.37719	-1006.37569	-1006.3741	-1006.35071	-1006.34885
67	-1006.37729	-1006.37582	-1006.37423	-1006.35054	-1006.34871
68	-1006.37736	-1006.37585	-1006.37426	-1006.35036	-1006.34857
69	-1006.37748	-1006.37601	-1006.37442	-1006.35016	-1006.34841
70	-1006.37759	-1006.37614	-1006.37455	-1006.34995	-1006.34824
71	-1006.37765	-1006.37618	-1006.37459	-1006.34972	-1006.34806
72	-1006.37776	-1006.37633	-1006.37474	-1006.34948	-1006.34786
73	-1006.37784	-1006.37642	-1006.37483	-1006.34922	-1006.34765
74	-1006.37793	-1006.37653	-1006.37494	-1006.34896	-1006.34742
75	-1006.378	-1006.37661	-1006.37502	-1006.3487	-1006.34718
76	-1006.37807	-1006.3767	-1006.37511	-1006.34846	-1006.34692
77	-1006.37814	-1006.37679	-1006.3752	-1006.34825	-1006.34666
78	-1006.3782	-1006.37688	-1006.37529	-1006.34807	-1006.3464
79	-1006.37826	-1006.37696	-1006.37537	-1006.34793	-1006.34616
80	-1006.37831	-1006.37703	-1006.37544	-1006.34783	-1006.34595
81	-1006.37836	-1006.37708	-1006.37549	-1006.34776	-1006.34577

82	-1006.3784	-1006.37712	-1006.37553	-1006.34771	-1006.34563
83	-1006.37844	-1006.37717	-1006.37558	-1006.34754	-1006.34553
84	-1006.37845	-1006.37716	-1006.37557	-1006.34771	-1006.34546
85	-1006.37851	-1006.37725	-1006.37566	-1006.34776	-1006.34541
86	-1006.37855	-1006.37731	-1006.37572	-1006.34783	-1006.34524
87	-1006.37857	-1006.37735	-1006.37576	-1006.34795	-1006.34541
88	-1006.3786	-1006.37742	-1006.37583	-1006.34812	-1006.34546
89	-1006.37863	-1006.37744	-1006.37585	-1006.34837	-1006.34553
90	-1006.37866	-1006.37748	-1006.37589	-1006.3487	-1006.34565
91	-1006.37868	-1006.3775	-1006.37591	-1006.34914	-1006.34582
92	-1006.37868	-1006.37749	-1006.3759	-1006.34971	-1006.34607
93	-1006.37866	-1006.37746	-1006.37587	-1006.3504	-1006.3464
94	-1006.37867	-1006.37746	-1006.37587	-1006.35124	-1006.34684
95	-1006.37869	-1006.37751	-1006.37592	-1006.35221	-1006.34741
96	-1006.37872	-1006.37756	-1006.37597	-1006.35332	-1006.3481
97	-1006.37871	-1006.37755	-1006.37596	-1006.35454	-1006.34894
98	-1006.37873	-1006.37759	-1006.376	-1006.35587	-1006.34991
99	-1006.37873	-1006.37758	-1006.37599	-1006.35728	-1006.35102
100	-1006.37873	-1006.37758	-1006.37599	-1006.35874	-1006.35224
101	-1006.37872	-1006.37756	-1006.37597	-1006.36021	-1006.35357
102	-1006.37871	-1006.37754	-1006.37595	-1006.36164	-1006.35498
103	-1006.37871	-1006.37754	-1006.37595	-1006.36298	-1006.35644
104	-1006.37869	-1006.37749	-1006.3759	-1006.36418	-1006.35791
105	-1006.37872	-1006.37755	-1006.37596	-1006.36518	-1006.35934
106	-1006.37873	-1006.37757	-1006.37598	-1006.36598	-1006.36068
107	-1006.37873	-1006.37757	-1006.37598	-1006.3666	-1006.36188
108	-1006.37873	-1006.37757	-1006.37598	-1006.36708	-1006.36288
109	-1006.37873	-1006.37756	-1006.37597	-1006.36746	-1006.36368
110	-1006.37874	-1006.37758	-1006.37599	-1006.36777	-1006.3643
111	-1006.37873	-1006.37756	-1006.37597	-1006.36801	-1006.36478
112				-1006.3682	-1006.36516
113				-1006.36833	-1006.36547
114				-1006.3684	-1006.36571
115				-1006.36856	-1006.3659
116				-1006.36866	-1006.36603
117				-1006.3687	-1006.3661
118				-1006.36885	-1006.36626
119				-1006.36895	-1006.36636
120				-1006.36903	-1006.3664
121				-1006.36909	-1006.36655
122				-1006.36914	-1006.36665
123				-1006.36925	-1006.36673
124				-1006.36932	-1006.36679

125				-1006.3694	-1006.36684
126				-1006.36947	-1006.36695
127				-1006.36954	-1006.36702
128				-1006.3696	-1006.3671
129				-1006.36966	-1006.36717
130				-1006.36972	-1006.36724
131				-1006.36977	-1006.3673
132				-1006.36982	-1006.36736
133				-1006.36988	-1006.36742
134				-1006.36992	-1006.36747
135				-1006.36997	-1006.36752
136				-1006.37001	-1006.36758
137				-1006.37006	-1006.36762
138				-1006.37009	-1006.36767
139				-1006.37013	-1006.36771
140				-1006.37015	-1006.36776
141				-1006.3702	-1006.36779
142				-1006.37023	-1006.36783
143				-1006.37026	-1006.36785
144				-1006.37029	-1006.3679
145				-1006.37031	-1006.36793
146				-1006.37034	-1006.36796
147				-1006.37037	-1006.36799
148				-1006.37039	-1006.36801
149				-1006.37042	-1006.36804
150				-1006.37044	-1006.36807
151				-1006.37047	-1006.36809
152				-1006.37049	-1006.36812
153				-1006.37051	-1006.36814
154				-1006.37054	-1006.36817
155				-1006.37056	-1006.36819
156				-1006.37058	-1006.36821
157				-1006.3706	-1006.36824
158				-1006.37063	-1006.36826
159				-1006.37065	-1006.36828
160				-1006.37067	-1006.3683
161				-1006.37069	-1006.36833
162				-1006.37072	-1006.36835
163				-1006.37074	-1006.36837
164				-1006.37076	-1006.36839
165				-1006.37078	-1006.36842
166				-1006.37081	-1006.36844
167				-1006.37083	-1006.36846

168				-1006.37085	-1006.36848
169				-1006.37087	-1006.36851
170				-1006.3709	-1006.36853
171				-1006.37092	-1006.36855
172				-1006.37094	-1006.36857
173				-1006.37096	-1006.3686
174				-1006.37099	-1006.36862
175				-1006.37101	-1006.36864
176				-1006.37103	-1006.36866
177				-1006.37105	-1006.36869
178				-1006.37108	-1006.36871
179				-1006.3711	-1006.36873
180				-1006.37112	-1006.36875
181				-1006.37114	-1006.36878
182					-1006.3688

Table S2 IRC transition state structures for the reaction of sulfate radical (SR) with phenol in the -X-axis electric field (calculated absolved energies)

(step)\EF strength (a.u.)	Total Energy (Hartree)				
	0	-0.0002	-0.0005	-0.001	-0.002
1	-1006.3587	-1006.35969	-1006.36119	-1006.36375	-1006.36494
2	-1006.3587	-1006.35968	-1006.36119	-1006.36373	-1006.36496
3	-1006.3587	-1006.35968	-1006.36118	-1006.3639	-1006.3651
4	-1006.3587	-1006.35968	-1006.36117	-1006.36374	-1006.36493
5	-1006.3587	-1006.35968	-1006.36115	-1006.36379	-1006.36498
6	-1006.35869	-1006.35967	-1006.36113	-1006.36388	-1006.36508
7	-1006.35869	-1006.35967	-1006.3611	-1006.36405	-1006.36525
8	-1006.35869	-1006.35966	-1006.36106	-1006.36428	-1006.36548
9	-1006.35868	-1006.35965	-1006.36103	-1006.36456	-1006.36576
10	-1006.35868	-1006.35964	-1006.36099	-1006.36485	-1006.36605
11	-1006.35867	-1006.35962	-1006.36094	-1006.36514	-1006.36634
12	-1006.35866	-1006.3596	-1006.36089	-1006.36541	-1006.36661
13	-1006.35864	-1006.35956	-1006.36084	-1006.36566	-1006.36686
14	-1006.35862	-1006.35952	-1006.3608	-1006.36589	-1006.36709
15	-1006.35858	-1006.35947	-1006.36086	-1006.3661	-1006.3673
16	-1006.35854	-1006.35942	-1006.36081	-1006.36629	-1006.36749
17	-1006.3585	-1006.35937	-1006.36091	-1006.36648	-1006.36768
18	-1006.35844	-1006.3593	-1006.36106	-1006.36665	-1006.36785
19	-1006.35839	-1006.35922	-1006.36127	-1006.36681	-1006.36801
20	-1006.35832	-1006.35915	-1006.36149	-1006.36697	-1006.36817
21	-1006.35824	-1006.35907	-1006.36172	-1006.36713	-1006.36834
22	-1006.35816	-1006.35901	-1006.36194	-1006.3673	-1006.3685

23	-1006.35806	-1006.35901	-1006.36215	-1006.36748	-1006.36868
24	-1006.35797	-1006.35902	-1006.36235	-1006.36769	-1006.36889
25	-1006.35788	-1006.35911	-1006.36253	-1006.36793	-1006.36913
26	-1006.35781	-1006.35926	-1006.36271	-1006.36823	-1006.36943
27	-1006.35778	-1006.35944	-1006.36287	-1006.36859	-1006.36979
28	-1006.35781	-1006.35963	-1006.36303	-1006.36903	-1006.37023
29	-1006.3579	-1006.35982	-1006.3632	-1006.36957	-1006.37077
30	-1006.35803	-1006.36001	-1006.36338	-1006.37021	-1006.37141
31	-1006.35819	-1006.36019	-1006.36358	-1006.37096	-1006.37217
32	-1006.35836	-1006.36035	-1006.36381	-1006.37181	-1006.37301
33	-1006.35853	-1006.36051	-1006.36409	-1006.37276	-1006.37396
34	-1006.3587	-1006.36067	-1006.36444	-1006.3738	-1006.375
35	-1006.35886	-1006.36083	-1006.36488	-1006.37491	-1006.37611
36	-1006.35901	-1006.361	-1006.36542	-1006.37606	-1006.37725
37	-1006.35916	-1006.36119	-1006.36608	-1006.37721	-1006.37841
38	-1006.35931	-1006.36142	-1006.36685	-1006.37831	-1006.37951
39	-1006.35948	-1006.36169	-1006.36775	-1006.37933	-1006.38054
40	-1006.35967	-1006.36202	-1006.36877	-1006.38021	-1006.38141
41	-1006.35988	-1006.36245	-1006.36989	-1006.38093	-1006.38213
42	-1006.36015	-1006.36298	-1006.3711	-1006.38149	-1006.38269
43	-1006.36048	-1006.36363	-1006.37236	-1006.38192	-1006.38313
44	-1006.36091	-1006.36441	-1006.37363	-1006.38228	-1006.38348
45	-1006.36144	-1006.36532	-1006.37485	-1006.38255	-1006.38375
46	-1006.36209	-1006.36635	-1006.37598	-1006.38276	-1006.38395
47	-1006.36287	-1006.3675	-1006.37695	-1006.38295	-1006.38415
48	-1006.36378	-1006.36873	-1006.37774	-1006.3831	-1006.3843
49	-1006.36483	-1006.37004	-1006.37834	-1006.3832	-1006.3844
50	-1006.36598	-1006.37136	-1006.3788	-1006.38327	-1006.38447
51	-1006.36724	-1006.37265	-1006.37918	-1006.3834	-1006.3846
52	-1006.36856	-1006.37385	-1006.37945	-1006.38349	-1006.38469
53	-1006.36991	-1006.37489	-1006.37964	-1006.38359	-1006.38479
54	-1006.37123	-1006.37575	-1006.37986	-1006.38367	-1006.38487
55	-1006.37246	-1006.37641	-1006.38002	-1006.38373	-1006.38493
56	-1006.37355	-1006.3769	-1006.38014	-1006.38382	-1006.38502
57	-1006.37444	-1006.37728	-1006.38022	-1006.38389	-1006.38509
58	-1006.37513	-1006.37761	-1006.38031	-1006.38396	-1006.38516
59	-1006.37566	-1006.37781	-1006.3804	-1006.38402	-1006.38522
60	-1006.37606	-1006.37796	-1006.38051	-1006.38409	-1006.38529
61	-1006.37634	-1006.37816	-1006.38061	-1006.38414	-1006.38534
62	-1006.37662	-1006.3783	-1006.38069	-1006.38418	-1006.38538
63	-1006.37676	-1006.3784	-1006.38077	-1006.38423	-1006.38543
64	-1006.37691	-1006.37845	-1006.38083	-1006.38427	-1006.38547
65	-1006.37709	-1006.37858	-1006.38092	-1006.3843	-1006.3855

66	-1006.37719	-1006.37869	-1006.38098	-1006.38434	-1006.38554
67	-1006.37729	-1006.37876	-1006.38105	-1006.38439	-1006.38559
68	-1006.37736	-1006.37887	-1006.38111	-1006.38443	-1006.38563
69	-1006.37748	-1006.37895	-1006.38117	-1006.38446	-1006.38566
70	-1006.37759	-1006.37904	-1006.38122	-1006.38449	-1006.38569
71	-1006.37765	-1006.37912	-1006.38127	-1006.38452	-1006.38572
72	-1006.37776	-1006.37919	-1006.38131	-1006.38454	-1006.38574
73	-1006.37784	-1006.37926	-1006.38134	-1006.38453	-1006.38573
74	-1006.37793	-1006.37933	-1006.38137	-1006.38454	-1006.38574
75	-1006.378	-1006.37939	-1006.38141	-1006.38455	-1006.38575
76	-1006.37807	-1006.37944	-1006.38145	-1006.3846	-1006.3858
77	-1006.37814	-1006.37949	-1006.38148	-1006.38461	-1006.38581
78	-1006.3782	-1006.37952	-1006.38151	-1006.38463	-1006.38583
79	-1006.37826	-1006.37956	-1006.38153	-1006.38464	-1006.38584
80	-1006.37831	-1006.37959	-1006.38152	-1006.38465	-1006.38585
81	-1006.37836	-1006.37964	-1006.38155	-1006.38466	-1006.38586
82	-1006.3784	-1006.37968	-1006.38156	-1006.38468	-1006.38588
83	-1006.37844	-1006.37971	-1006.3816	-1006.38469	-1006.38589
84	-1006.37845	-1006.37974	-1006.38161	-1006.3847	-1006.3859
85	-1006.37851	-1006.37977	-1006.38162		
86	-1006.37855	-1006.37979	-1006.38162		
87	-1006.37857	-1006.37979	-1006.38163		
88	-1006.3786	-1006.37978	-1006.38163		
89	-1006.37863	-1006.37982	-1006.38164		
90	-1006.37866	-1006.37984	-1006.38164		
91	-1006.37868	-1006.37986	-1006.38165		
92	-1006.37868	-1006.37987	-1006.38165		
93	-1006.37866	-1006.37986	-1006.38165		
94	-1006.37867	-1006.37988	-1006.38166		
95	-1006.37869	-1006.37987	-1006.38167		
96	-1006.37872	-1006.37988	-1006.38167		
97	-1006.37871	-1006.37987	-1006.38168		
98	-1006.37873	-1006.37987	-1006.38168		
99	-1006.37873	-1006.37988	-1006.38169		
100	-1006.37873	-1006.37988			
101	-1006.37872	-1006.37988			
102	-1006.37871	-1006.37988			
103	-1006.37871	-1006.37988			
104	-1006.37869	-1006.37989			
105	-1006.37872	-1006.37989			
106	-1006.37873	-1006.37989			
107	-1006.37873	-1006.37989			
108	-1006.37873	-1006.37989			

109	-1006.37873	-1006.3799			
110	-1006.37874	-1006.3799			
111	-1006.37873	-1006.3799			

Table S3 Atomic coordinate position without an external electric field

Atomic number	Atom	x(Bohr)	y(Bohr)	z(Bohr)
1	C	2.226822	0.067588	-2.106271
2	C	2.884209	-2.472299	-1.872258
3	C	4.645008	-3.242961	-0.069689
4	C	5.753649	-1.44039	1.507281
5	C	5.124567	1.106868	1.289064
6	C	3.357849	1.856497	-0.523403
7	O	2.66604	4.314894	-0.837703
8	H	1.99107	-3.8527	-3.098447
9	H	5.146149	-5.222378	0.111485
10	H	7.125079	-2.015301	2.921002
11	H	5.992832	2.506289	2.515862
12	H	3.512783	5.37428	0.384106
13	S	-3.80793	-0.204209	0.235917
14	O	-5.557794	-0.03517	2.427733
15	O	-3.713741	-2.709061	-0.951596
16	O	-1.286929	0.204372	1.836885
17	O	-4.046571	1.886343	-1.573819
18	H	0.844861	0.691443	-3.487748

Table S4 Atomic coordinates under an externally applied negative electric field of 0.0002 a.u..

Atomic number	Atom	x(Bohr)	y(Bohr)	z(Bohr)
1	C	2.177671	0.052606	2.088215
2	C	2.830869	-2.490662	1.875767
3	C	4.612294	-3.27536	0.100152
4	C	5.746701	-1.483747	1.471474
5	C	5.122812	1.066357	1.274367
6	C	3.33589	1.830639	0.511928
7	O	2.649148	4.292658	0.806278
8	H	1.919437	-3.861996	3.098788
9	H	5.1115	-5.256712	0.06345
10	H	7.135367	-2.069603	2.863352
11	H	6.012678	2.45674	2.495614
12	H	3.525848	5.345495	0.400058
13	S	-3.864772	-0.174004	0.239812
14	O	-5.601524	0.000681	2.440994
15	O	-3.810112	-2.670911	0.968121
16	O	-1.32613	0.188342	1.826152
17	O	-4.086874	1.933172	1.553117

18	H	0.783574	0.688451	3.451915
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Table S5 Atomic coordinates under an externally applied negative electric field of 0.0005 a.u..

Atomic number	Atom	x(Bohr)	y(Bohr)	z(Bohr)
1	C	2.117198	0.050597	-1.999073
2	C	2.755965	-2.498144	-1.792593
3	C	4.602274	-3.283944	-0.086921
4	C	5.817998	-1.48925	1.420161
5	C	5.210113	1.065115	1.228108
6	C	3.358345	1.831605	-0.489318
7	O	2.681171	4.296426	-0.777625
8	H	1.781551	-3.87015	-2.965262
9	H	5.091776	-5.268	0.072449
10	H	7.259645	-2.076579	2.756353
11	H	6.165604	2.456485	2.397578
12	H	3.640077	5.356573	0.35813
13	S	-3.880783	-0.168956	0.222816
14	O	-5.635392	-0.020576	2.409468
15	O	-3.828484	-2.646055	-1.026211
16	O	-1.340345	0.15537	1.822813
17	O	-4.079337	1.967448	-1.539846
18	H	0.679707	0.6903	-3.315105

Table S6 Atomic coordinates under an externally applied negative electric field of 0.001 a.u..

Atomic number	Atom	x(Bohr)	y(Bohr)	z(Bohr)
1	C	2.046213	0.03142	-1.85887
2	C	2.697297	-2.522092	-1.674811
3	C	4.622477	-3.296219	-0.062066
4	C	5.916788	-1.490165	1.373256
5	C	5.307767	1.062752	1.200249
6	C	3.375304	1.824117	-0.429201
7	O	2.693315	4.281302	-0.707504
8	H	1.661755	-3.896285	-2.790307
9	H	5.122115	-5.278404	0.085081
10	H	7.423826	-2.074455	2.636277
11	H	6.327494	2.457353	2.309049
12	H	3.725792	5.355788	0.348912
13	S	-3.82638	-0.154708	0.19067
14	O	-5.551627	-0.008353	2.399719
15	O	-3.83198	-2.624917	-1.084065
16	O	-1.22672	0.137351	1.697865
17	O	-4.062019	1.991607	-1.563725
18	H	0.576041	0.67358	-3.136427

Table S7 Atomic coordinates under an externally applied negative electric field of 0.002 a.u..

Atomic number	Atom	x(Bohr)	y(Bohr)	z(Bohr)
1	C	1.302327	-0.089995	-0.736587
2	C	2.335307	-2.721963	-0.711292
3	C	4.719618	-3.253428	0.097529
4	C	6.400968	-1.304148	0.86927
5	C	5.620228	1.240674	0.773813
6	C	3.2326	1.850513	-0.025613
7	O	2.354159	4.236868	-0.245913
8	H	1.038954	-4.197096	-1.301351
9	H	5.364285	-5.201126	0.145797
10	H	8.288565	-1.764317	1.516015
11	H	6.918187	2.739379	1.309798
12	H	3.635617	5.444135	0.244411
13	S	-3.628826	-0.1603	-0.057835
14	O	-5.165361	-0.081489	2.252028
15	O	-3.647152	-2.605466	-1.392998
16	O	-0.754985	0.122751	1.100056
17	O	-3.976897	2.019675	-1.755357
18	H	0.504461	0.405827	-2.590984

Table S8 Atomic coordinates under an externally applied positive electric field of 0.0002 a.u..

Atomic number	Atom	x(Bohr)	y(Bohr)	z(Bohr)
1	C	2.273247	0.069498	-2.129798
2	C	2.912682	-2.475824	-1.910659
3	C	4.650642	-3.27273	-0.096484
4	C	5.754203	-1.490525	1.506738
5	C	5.142861	1.062327	1.303073
6	C	3.398574	1.837849	-0.520336
7	O	2.72521	4.303213	-0.821367
8	H	2.022277	-3.840739	-3.156756
9	H	5.13626	-5.256979	0.074138
10	H	7.107198	-2.085564	2.929506
11	H	6.007202	2.44609	2.549006
12	H	3.546461	5.343796	0.434159
13	S	-3.771919	-0.181133	0.240911
14	O	-5.523159	-0.01634	2.433301
15	O	-3.688775	-2.679434	-0.960979
16	O	-1.257607	0.2051	1.852678
17	O	-3.997839	1.921528	-1.555828
18	H	0.906098	0.712353	-3.517599

Table S9 Atomic coordinates under an externally applied positive electric field of 0.0005 a.u..

Atomic number	Atom	x(Bohr)	y(Bohr)	z(Bohr)
1	C	2.354502	0.083365	-2.157881
2	C	2.985255	-2.462453	-1.928199
3	C	4.690901	-3.263089	-0.08469
4	C	5.768779	-1.483674	1.538217
5	C	5.1643	1.07034	1.325245
6	C	3.452278	1.848783	-0.527224
7	O	2.785574	4.315483	-0.836262
8	H	2.111853	-3.825964	-3.187463
9	H	5.168101	-5.248689	0.094256
10	H	7.094321	-2.081588	2.985899
11	H	6.005298	2.452541	2.590196
12	H	3.570105	5.351039	0.445933
13	S	-3.683468	-0.193135	0.238763
14	O	-5.446895	-0.03242	2.423387
15	O	-3.574724	-2.69569	-0.950824
16	O	-1.189776	0.219925	1.870014
17	O	-3.915229	1.900204	-1.567222
18	H	1.007117	0.727681	-3.56391

Table S10 Atomic coordinates under an externally applied positive electric field of 0.001 a.u..

Atomic number	Atom	x(Bohr)	y(Bohr)	z(Bohr)
1	C	2.600915	0.113451	-2.232526
2	C	3.206534	-2.434409	-1.974291
3	C	4.810125	-3.246342	-0.044838
4	C	5.807817	-1.475411	1.636286
5	C	5.224213	1.081543	1.397268
6	C	3.614359	1.869992	-0.540642
7	O	2.972301	4.340439	-0.877712
8	H	2.390374	-3.792933	-3.276541
9	H	5.264532	-5.235225	0.156921
10	H	7.049848	-2.081984	3.152915
11	H	5.997048	2.457878	2.711246
12	H	3.647403	5.362478	0.475514
13	S	-3.443696	-0.215572	0.228558
14	O	-5.241347	-0.064062	2.393954
15	O	-3.285704	-2.727307	-0.934233
16	O	-1.009414	0.253243	1.908362
17	O	-3.690763	1.857074	-1.597478
18	H	1.325074	0.764399	-3.70061

Table S11 Atomic coordinates under an externally applied positive electric field of 0.0002 a.u..

Atomic number	Atom	x(Bohr)	y(Bohr)	z(Bohr)
1	C	3.278114	0.293082	-2.472466
2	C	3.79137	-2.275531	-2.244126
3	C	5.093547	-3.207691	-0.145859
4	C	5.877737	-1.534055	1.733139
5	C	5.378841	1.045018	1.526746
6	C	4.070237	1.950113	-0.578332
7	O	3.521459	4.449792	-0.889006
8	H	3.134884	-3.561398	-3.701722
9	H	5.466879	-5.215797	0.032538
10	H	6.87442	-2.232669	3.385601
11	H	5.970689	2.345619	3.002258
12	H	3.926456	5.381463	0.626927
13	S	-2.814634	-0.283842	0.264245
14	O	-4.861071	-0.114179	2.273492
15	O	-2.571325	-2.833591	-0.792518
16	O	-0.715565	0.28615	2.20058
17	O	-3.015337	1.718703	-1.639147
18	H	2.219871	1.032032	-4.066193