Supplementary Materials

Is It Possible to Restrain OER on Simple Carbon Electrodes to Efficiently Electrooxidize Organic Pollutants?

Marija Ječmenica Dučić [1], Danka Aćimović [1], Branislava Savić [1], Lazar Rakočević [2], Marija Simić [1], Tanja Brdarić [1] and Dragana Vasić Anićijević [1,*]

[1] University of Belgrade, Vinča Institute of Nuclear Sciences-National Institute of the Republic of Serbia, Department of Physical Chemistry, Mike Petrovića Alasa 12–14, 11001 Belgrade, Serbia
[2] University of Belgrade, Vinča Institute of Nuclear Sciences-National Institute of the Republic of Serbia, Department of Atomics Physics, Mike Petrovića Alasa 12–14, 11001 Belgrade, Serbia
* Correspondence: draganav@vin.bg.ac.rs; Tel.: +381-11-34-08-287

Table S1. Atomic percents measured by XPS.

CNT Pb		
C 1s	82.9	%
O 1s	11.1	%
Pb 4f	6	%
CNT Sn		
C 1s	93.8	%
O 1s	5.1	%
Sn 3d	1.1	%
CNT		
C 1s	98.7	%
O 1s	1.3	%

Table S2. Fukui indices of Rhodamine B molecule.

	Nucleophilicity				Radical Attack			
	RhB Atom	q(N)	q(N − 1)	Fa-	Rhb Atom	q(N + 1)	q(N − 1)	Fa0
1	O	7.857322	7.74038	0.116942	O	7.906223	7.74038	0.165843
2	O	7.670466	7.421019	0.249447	O	7.747194	7.421019	0.326175
3	O	7.637462	7.626688	0.010774	O	7.645222	7.626688	0.018534
4	N	7.446052	7.294789	0.151263	N	7.499211	7.294789	0.204422
5	N	6.975949	7.485839	−0.50989	N	6.930749	7.485839	−0.55509
6	C	1.132712	1.237361	−0.10465	C	1.126596	1.237361	−0.11077
7	C	4.094932	4.064295	0.030637	C	4.103981	4.064295	0.039686
8	C	4.071462	4.054048	0.017414	C	4.087168	4.054048	0.03312
9	C	3.998633	3.999706	−0.00107	C	4.011458	3.999706	0.011752
10	C	4.085829	4.087221	−0.00139	C	4.090176	4.087221	0.002955
11	C	4.007695	4.0054	0.002295	C	4.011354	4.0054	0.005954
12	C	4.046196	4.044938	0.001258	C	4.079576	4.044938	0.034638
13	C	4.071093	4.069466	0.001627	C	4.073752	4.069466	0.004286
14	C	4.018033	4.043469	−0.02544	C	4.023992	4.043469	−0.01948
15	C	4.059778	4.01796	0.041818	C	4.056647	4.01796	0.038687
16	C	3.260852	3.320457	−0.05961	C	3.215158	3.320457	−0.1053
17	C	3.217452	3.298414	−0.08096	C	3.179920	3.298414	−0.11849
18	C	3.677878	3.427324	0.250554	C	3.643711	3.427324	0.216387
19	C	3.691415	3.438835	0.25258	C	3.732133	3.438835	0.293298
20	C	4.054983	4.039877	0.015106	C	4.074325	4.039877	0.034448
21	C	4.079402	4.065299	0.014103	C	4.090166	4.065299	0.024867
22	C	3.955236	3.953486	0.00175	C	3.979989	3.953486	0.026503
23	C	4.000374	3.999982	0.000392	C	4.039235	3.999982	0.039253
24	C	4.01917	3.992409	0.026761	C	4.041488	3.992409	0.049079
25	C	2.479919	2.487303	−0.00738	C	2.470000	2.487303	−0.0173
26	C	4.020836	4.014758	0.006078	C	3.999273	4.014758	−0.01548
27	C	3.030975	3.021861	0.009114	C	3.092706	3.021861	0.070845
28	C	2.631027	2.604319	0.026708	C	2.691442	2.604319	0.087123
29	C	3.326335	3.304751	0.021584	C	3.325081	3.304751	0.02033
30	C	4.787271	4.770424	0.016847	C	4.780000	4.770424	0.009576
31	C	3.970301	3.964803	0.005498	C	3.990442	3.964803	0.025639
32	C	4.019869	4.015367	0.004502	C	4.017893	4.015367	0.002526
33	C	3.958548	3.956734	0.001814	C	3.995756	3.956734	0.039022
34	H	0.92037	0.89109	0.02928	H	0.952720	0.89109	0.06163
35	H	0.963422	0.928827	0.034595	H	0.994867	0.928827	0.06604
36	H	0.874841	0.862776	0.012065	H	0.893311	0.862776	0.030535
37	H	0.950257	0.926371	0.023886	H	0.970004	0.926371	0.043633
38	H	0.972138	0.968097	0.004041	H	0.970997	0.968097	0.0029
39	H	0.958419	0.942727	0.015692	H	0.969153	0.942727	0.026426
40	H	1.006117	0.983609	0.022508	H	1.022024	0.983609	0.038415
41	H	0.973461	0.973067	0.000394	H	0.971908	0.973067	−0.00116
42	H	0.995152	0.980892	0.01426	H	1.005080	0.980892	0.024188
43	H	0.97336	0.959972	0.013388	H	0.997111	0.959972	0.037139
44	H	0.982663	0.972234	0.010429	H	0.997771	0.972234	0.025537
45	H	0.924575	0.924899	−0.00032	H	0.924829	0.924899	-7×10^{-5}
46	H	0.932392	0.914566	0.017826	H	0.956409	0.914566	0.041843
47	H	0.984957	0.974993	0.009964	H	0.997832	0.974993	0.022839
48	H	0.954584	0.953993	0.000591	H	0.956705	0.953993	0.002712
49	H	0.983982	0.925903	0.058079	H	0.995835	0.925903	0.069932
50	H	0.976985	0.952641	0.024344	H	0.995835	0.952641	0.043194
51	H	0.96807	0.953441	0.014629	H	0.975736	0.953441	0.022295
52	H	0.973857	0.950756	0.023101	H	0.988661	0.950756	0.037905
53	H	0.991473	0.976716	0.014757	H	1.001558	0.976716	0.024842
54	H	0.947746	0.940559	0.007187	H	0.961080	0.940559	0.020521
55	H	0.971623	0.95299	0.018633	H	0.997012	0.95299	0.044022
56	H	0.952402	0.946078	0.006324	H	0.964061	0.946078	0.017983
57	H	0.929275	0.91518	0.014095	H	0.952839	0.91518	0.037659
58	H	0.950161	0.919396	0.030765	H	0.980346	0.919396	0.06095
59	H	0.93309	0.904368	0.028722	H	0.970795	0.904368	0.066427

60	H	0.933681	0.92346	0.010221	H	0.953662	0.92346	0.030202
61	H	0.918723	0.911726	0.006997	H	0.948127	0.911726	0.036401
62	H	0.938901	0.917584	0.021317	H	0.959243	0.917584	0.041659
63	H	0.907826	0.882045	0.025781	H	0.943425	0.882045	0.06138

C-atoms 18 and 19, which are identified as the most reactive carbon atoms according to the indices, belong to ethyl groups bound to N – heteroatoms. **NOTE:** Although reactive, oxygen heteroatoms were not taken into consideration in cleavage site prediction, since their reactivity does not contribute to the cleavage of carbon chain.

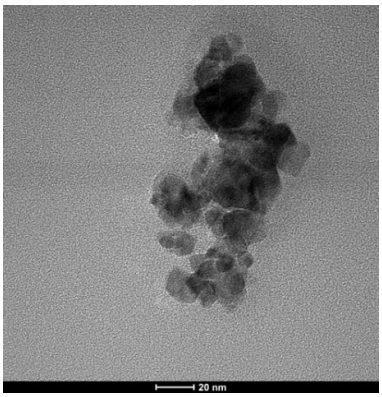

Figure S1. TEM micrograph of bare SnO_2 powder.