

Supplement

Lead Oxide-Modified Graphite Electrodes for Electrochemical Degradation of Congo Red Dye in Aqueous Solution

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Table S1 Fukui indices of CR dye

Atom	Fukui(⁰)	Fukui(+)	Fukui(-)
C-1	0.025	0.026	0.025
C-2	0.015	0.013	0.017
C-3	0.009	0.012	0.007
C-4	0.007	0.008	0.006
C-5	0.015	0.015	0.016
C-6	0.021	0.019	0.023
C-7	0.022	0.022	0.023
C-8	0.016	0.007	0.025
C-9	0.008	0.007	0.008
C-10	0.020	0.014	0.027
N-11	0.031	0.022	0.040
S-12	0.006	0.004	0.007
N-13	0.031	0.042	0.020
N-14	0.033	0.034	0.032
C-15	0.015	0.014	0.016
C-16	0.016	0.017	0.015
C-17	0.015	0.014	0.016
C-18	0.019	0.017	0.020
C-19	0.016	0.017	0.016
C-20	0.019	0.018	0.019
C-21	0.014	0.017	0.011
C-22	0.016	0.018	0.014
C-23	0.017	0.019	0.015
C-24	0.016	0.014	0.018
C-25	0.014	0.016	0.012
C-26	0.013	0.013	0.013
N-27	0.028	0.037	0.020
N-28	0.030	0.042	0.017
C-29	0.012	0.007	0.016
C-30	0.019	0.021	0.017
C-31	0.006	0.008	0.004

Table S2 Fukui indices of CR dye (continued)

Atom	Fukui(⁰)	Fukui(⁻)	Fukui(⁺)
C-32	0.009	0.012	0.006
C-33	0.017	0.014	0.020
C-34	0.008	0.009	0.006
H-35	0.015	0.015	0.015
H-36	0.009	0.009	0.010
H-37	0.009	0.009	0.009
H-38	0.014	0.013	0.015
H-39	0.007	0.006	0.008
H-40	0.012	0.009	0.014
H-41	0.015	0.013	0.018
H-42	0.010	0.011	0.009
H-43	0.010	0.010	0.011
H-44	0.011	0.011	0.011
H-45	0.013	0.013	0.013
H-46	0.010	0.011	0.009
H-47	0.012	0.013	0.012
H-48	0.009	0.010	0.009
H-49	0.009	0.009	0.008
H-50	0.007	0.007	0.006
C-51	0.013	0.013	0.013
H-52	0.008	0.008	0.007
C-53	0.023	0.026	0.020
H-54	0.014	0.015	0.012
C-55	0.018	0.019	0.017
H-56	0.012	0.013	0.011
C-57	0.013	0.014	0.012
H-58	0.008	0.008	0.007
S-59	0.006	0.006	0.007
O-60	0.015	0.015	0.015
O-61	0.011	0.011	0.012
O-62	0.008	0.008	0.009
O-63	0.020	0.016	0.023

Table S2 Identified degradation intermediates from the GC-MS analysis

Code	Compounds
A	Congo Red
B	cis-2,4-Dimethylthiane (Sulphonamide)
C	Squalene
D	Phthalic anhydride
E	Z,Z-6,25-Tetratriactontadien-2-one
F	9 12-octadecadienoic acid (z)-methyl ester
G	5-Hydroxymethylfurfural (Cyclic aldehyde)
H	Cyclohexene 4-(4-ethylcyclohexyl) -1-pentyl (Aldehyde)
I	Hexadecanoic acid methyl ester (Methyl ester)
J	Propanoic acid 2,3-dihydroxy- (Carboxylic Acid)
K	Dodecane (Alkane)
L	Propanenitrile, 2-hydroxy-
M	1-Propanol, 2-methyl-1-propanol (Primary alcohol)

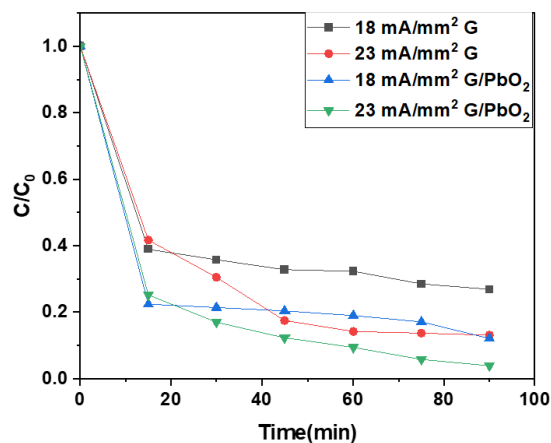


Fig. S1 Electrochemical degradation profile of CR dye by unmodified and PbO₂ modified graphite electrodes at different current densities (dye conc = 30 mg/L, electrolyte concentration = 1 M KCl, voltage = 25 V, pH = 7, T = 30 °C)

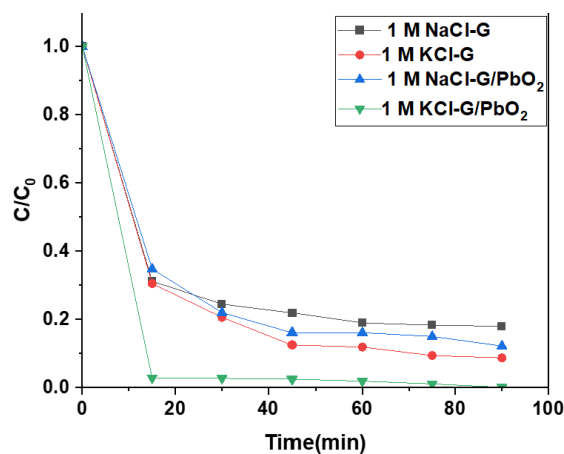


Fig. S2 Electrochemical degradation profile of CR dye by unmodified and PbO₂ modified graphite electrodes in different supporting electrolytes (dye conc = 30 mg/L, electrolyte concentration = 1 M, voltage = 30 V, current density = 23 mA/mm, pH = 7, T = 30 °C)

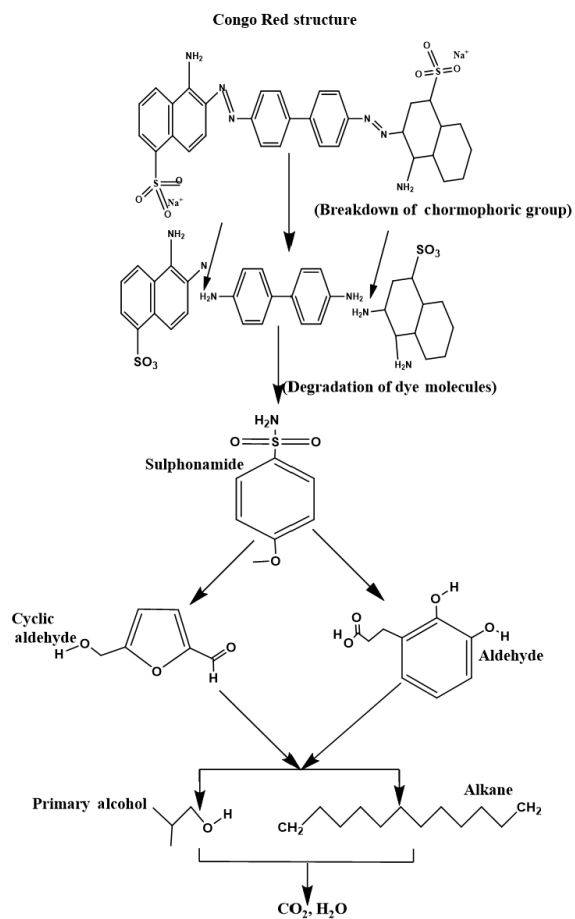


Fig. S3 Degradation pathway of CR dye in aqueous solution

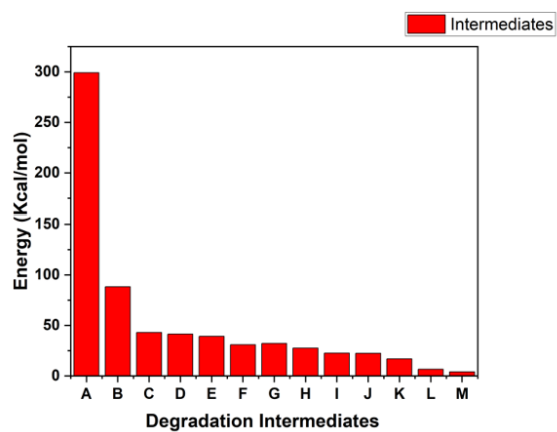


Fig. S4 Isothermal energy of degradation intermediates listed in Table S2 at 30 °C