Mechanistic inference on the roles of oxygenic functional groups to activate peroxymonosulfates in graphene for advanced oxidation

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Based on the reported studies, the kinetic of BPA degradation was evaluated by pseudo-first order kinetics given in Eq (1).

$$In\frac{C_t}{C_0} = -k_{obs}t$$

Where C_t is the BPA concentration at actual time (t), C_0 is the initial BPA concentration, k_{obs} is the rate constant and k_{SA} is the surface area normalized first order rate constant.

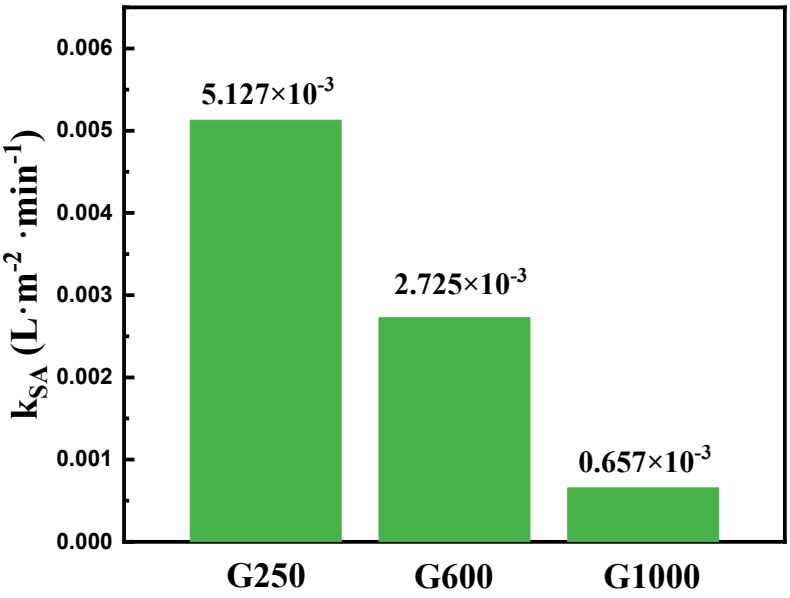


Fig. S1. Comparison of the k_{SA} values for various materials.

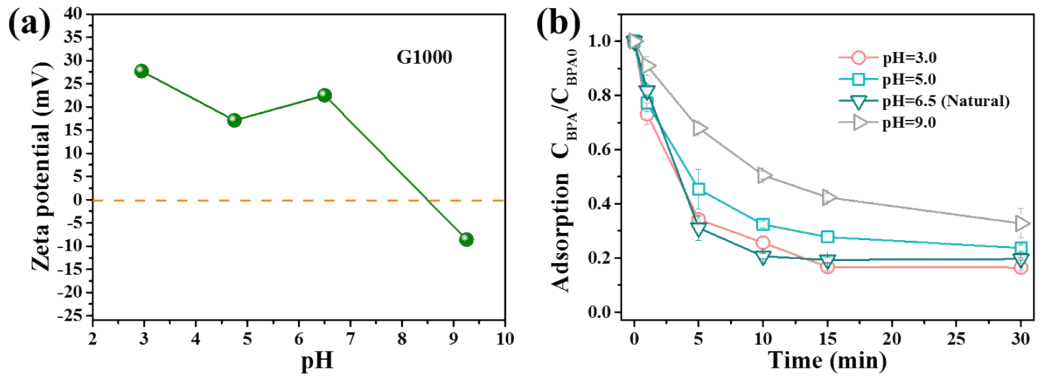


Fig. S2. The zeta potential of G1000 (a) and the adsorption of BPA (b) at different pH values. Reaction conditions: [BPA] = 19 mg L-1, [catalyst] = 0.1 g L-1, T = 298 K.

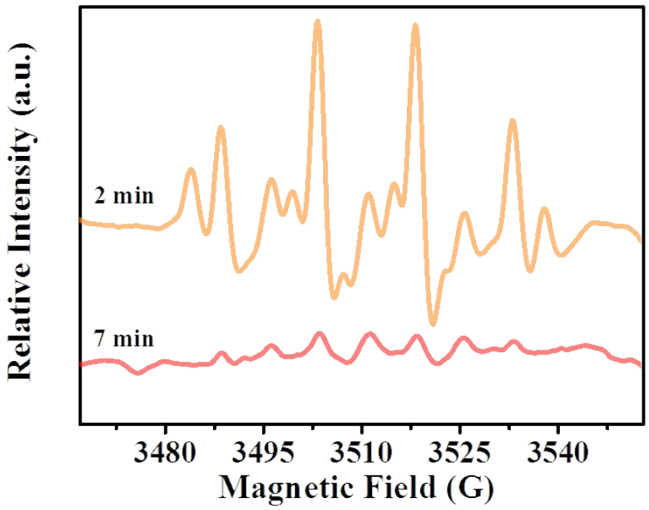


Fig. S3. EPR measurements with the addition of DMPO after 2 min and 7 min in the G1000/PMS system.

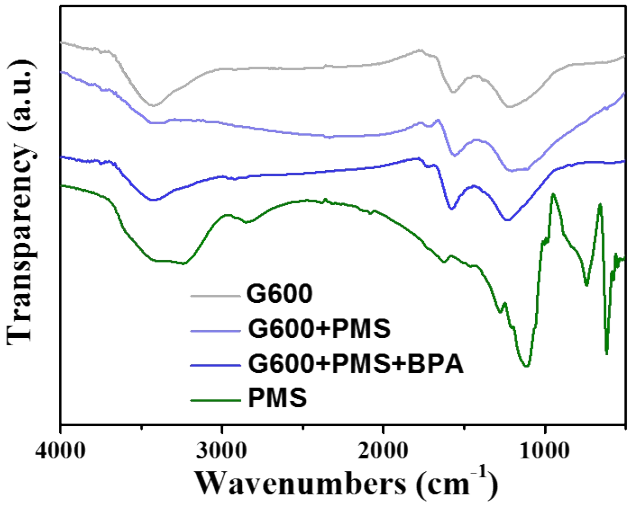


Fig. S4. FTIR spectra of G600 in different systems.

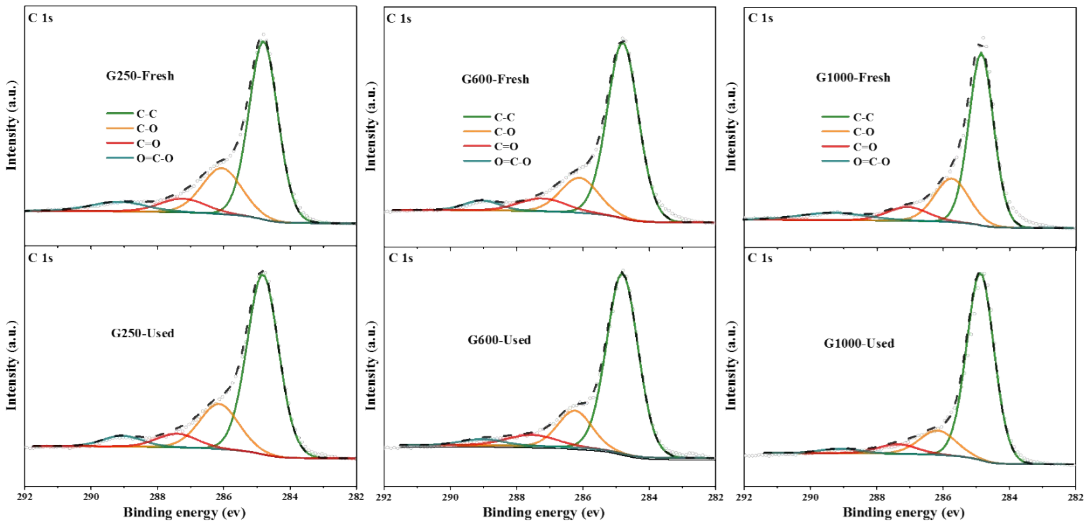


Fig. S5. High-resolution XPS spectra of C 1s of G250, G600 and G1000 before and after reactions.

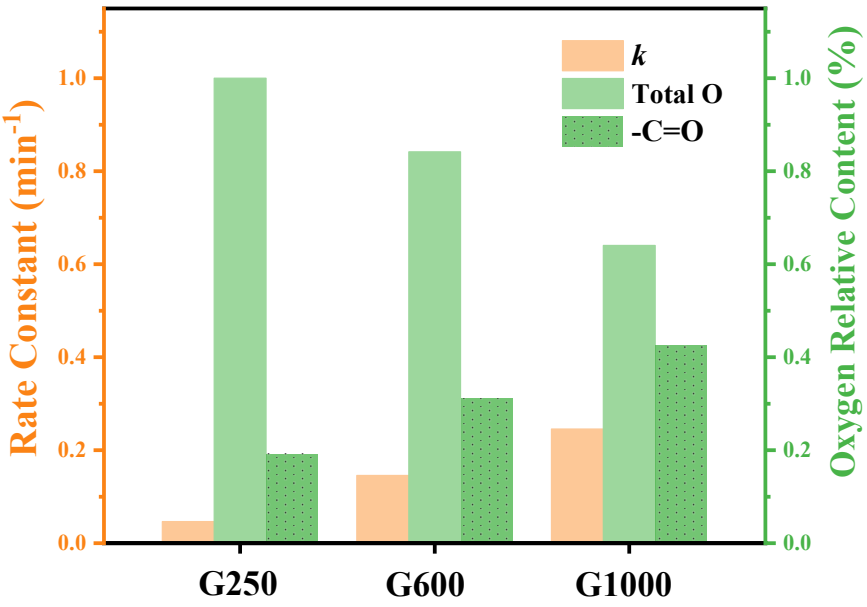


Fig. S6. The correlation between oxygen species content with rate constant.

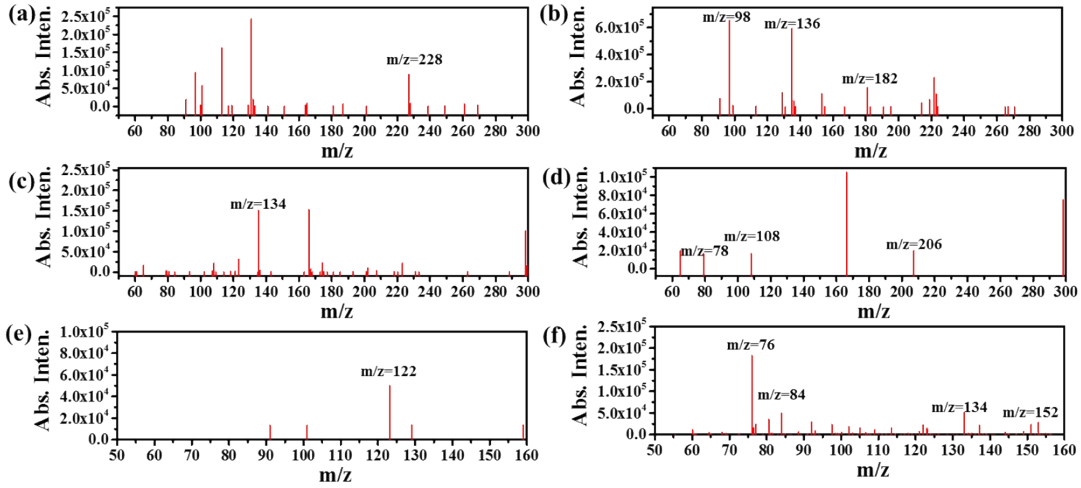
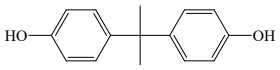
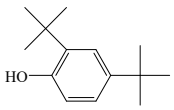
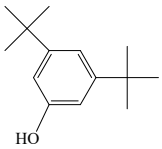
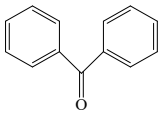
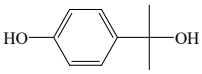
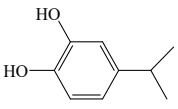
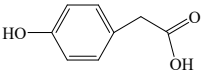
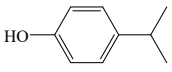
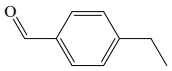
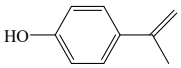
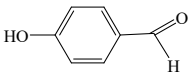
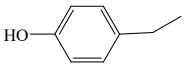
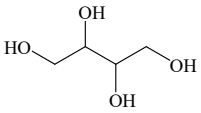
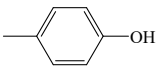
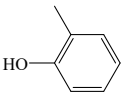
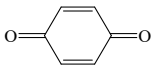
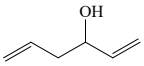
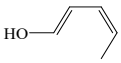
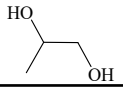


Fig. S7. (a)~(f) Mass spectrum of BPA degraded intermediates identified by LC-MS. Experimental conditions: [PMS] = 2.0 mM, [BPA] = 19 mg/L, [Catalyst] = 0.10 g/L, T = 298 K.

Table S1. Possible intermediates of BPA degradation.

No.	Tentative structure	Molecular formula	Molecular weight (m/z)
1		$C_{15}H_{16}O_2$	228
2		$C_{14}H_{22}O$	206
3		$C_{14}H_{22}O$	206
4		$C_{13}H_{10}O$	182
5		$C_9H_{12}O_2$	152
6		$C_9H_{12}O_2$	152
7		$C_8H_8O_3$	152
8		$C_9H_{12}O$	136

9		$C_9H_{10}O$	134
10		$C_9H_{10}O$	134
11		$C_7H_6O_2$	122
12		$C_8H_{10}O$	122
13		$C_4H_{10}O_4$	122
14		C_7H_8O	108
15		C_7H_8O	108
16		$C_6H_4O_2$	108
17		$C_6H_{10}O$	98
18		C_5H_8O	84
19		C_6H_6	78
20		$C_3H_8O_2$	76

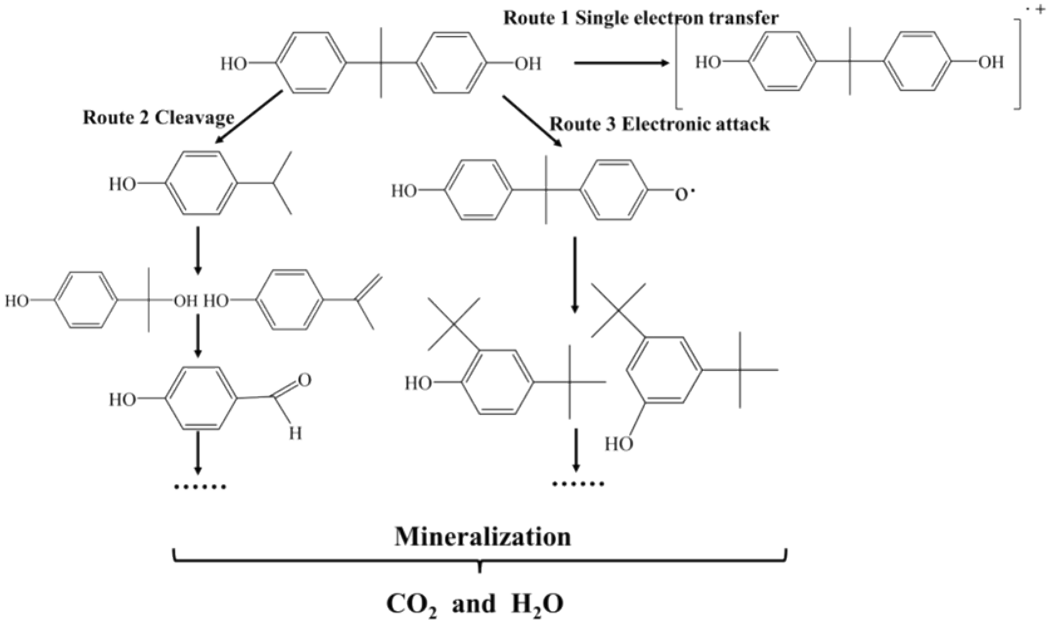


Fig. S8. The potential degradation pathway of BPA.

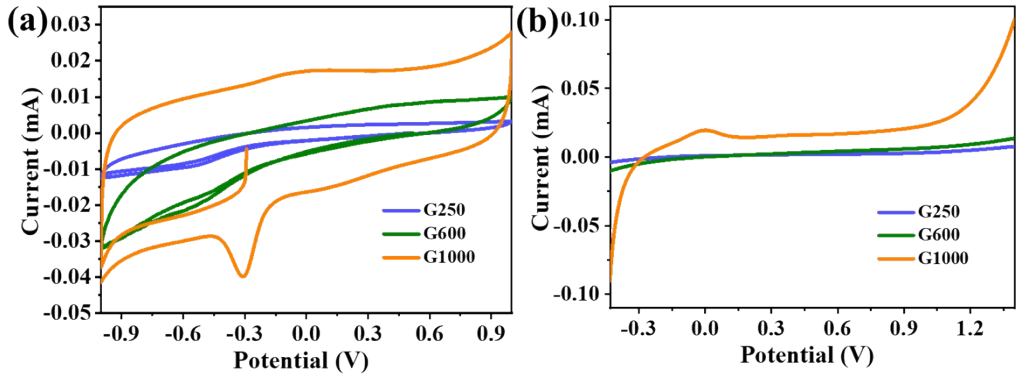


Fig. S9. (a) CVs of G250, G600 and G1000 at the rang from -0.9 to 0.9 V vs. Ag/AgCl; (b) LSV curves of G250, G600 and G1000.