[Supporting Information]

Photoenhanced Oxidation of C_{60} Aggregates (nC_{60}) by Free Chlorine in Water

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Calculation of chlorination reaction constants in Table 1:

As described by Equations (4) - (7) in the main text, the overall oxidation reaction of nC_{60} under aerobic and anaerobic conditions can be expressed as Equation (8) and (9) respectively, which can be further understood with Equation S1 and S2:

$$\ln\frac{F}{F_0} + k_1 t = k_{uv}\frac{([Cl_2]_0 - k_3 t)^2 - [Cl_2]_0^{\,2}}{2k_3} \quad \text{(Aerobic)} \qquad \text{(S1)}$$

$$\ln\frac{F}{F_0} = k_{uv}\frac{([Cl_2]_0 - k_3 t)^2 - [Cl_2]_0^{\,2}}{2k_3} \quad \text{(Anaerobic)} \qquad \text{(S2)}$$

Here, k_{UV} represents the oxychlorination reaction of nC_{60} by free chlorine and the rate constants for nC_{60} and oxygen (k_1) can be derived from control experiments with no free chlorine under aerobic conditions (Fig. 1b). Initial chlorine concentration ($[Cl]_0$) and degradation rate constants (k_3) were identified through chlorine concentration monitored during the reaction (Fig. S1). Thus, the rate constants between nC_{60} and free chlorine under UV irradiation can be derived from Equation S1 and S2 (with known variables: k_1, k_3, $[Cl_2]_0$), which is shown in Fig. S2 as an example.

Free chlorine photodecomposition and subsequent reactions in water:[1-6]

$HOCl\ (hv) \rightarrow \bullet OH + Cl\bullet$ (S3)

$OCl^-\ (hv) \rightarrow O_2\bullet^- + Cl\bullet$ (S4)

$Cl\bullet + OCl^-\ (HOCl\text{-}) \rightarrow ClO\bullet + Cl^-\ (HCl^-)$ (S5)

$\bullet OH + OCl^-\ (HOCl) \rightarrow ClO\bullet + OH^-\ (H_2O)$ (S6)

$Cl\bullet + Cl\text{-} \rightarrow Cl_2\bullet^-$ (S7)

$Cl_2O\ (hv) \rightarrow Cl\bullet + ClO\bullet$ (S8)

$Cl\bullet + Cl_2O \rightarrow Cl_2 + ClO\bullet$ (S9)

$Cl_2O\ (hv) \rightarrow Cl_2 + O\ (^3P)$ (S10)

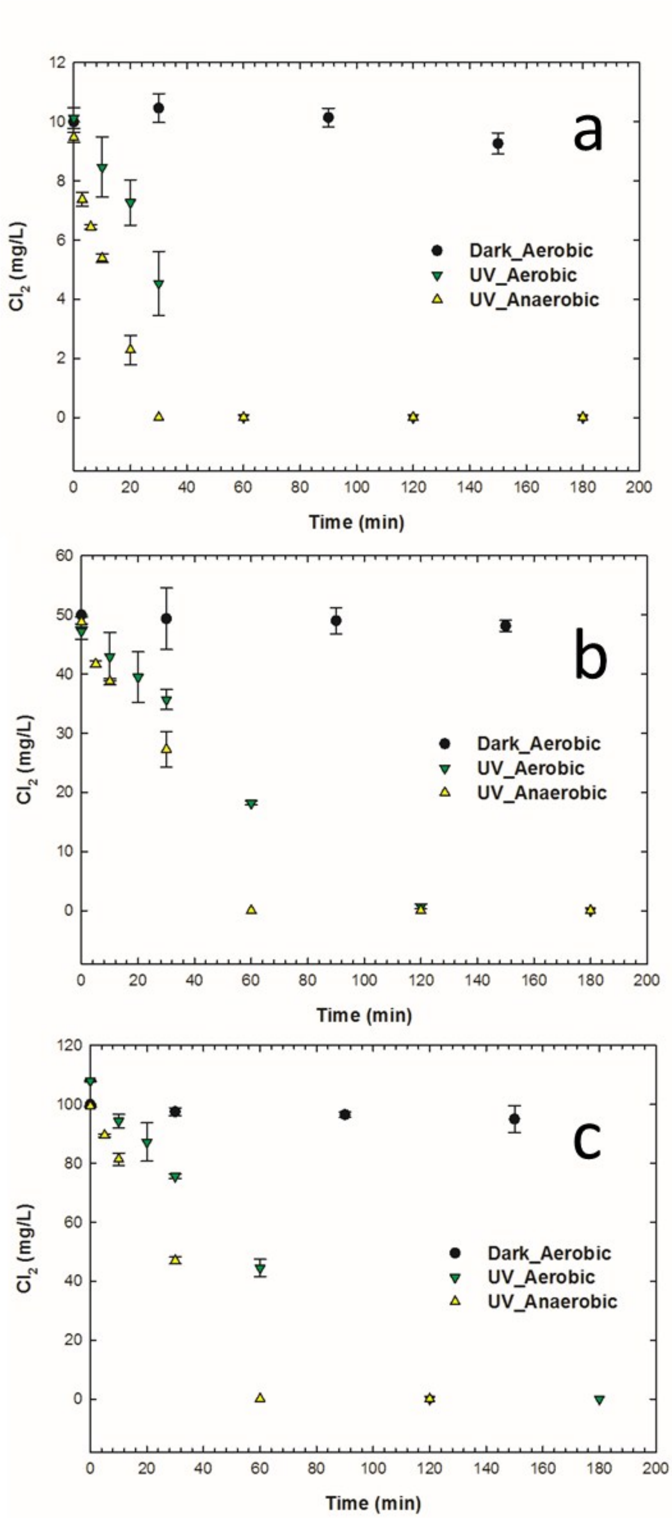

Fig. S1 Free chlorine concentrations during the reactions with different conditions: (a) 10 mg/L Cl_2; (b) 50 mg/L Cl_2; (c) 100 mg/L Cl_2.

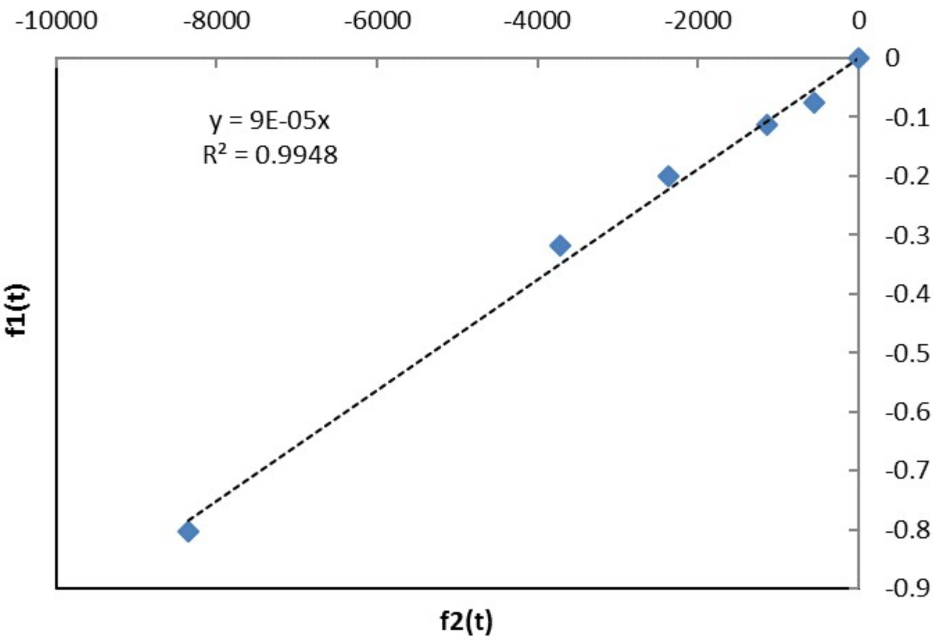

Fig. S2 Linear relationship between $f_1(t)$ and $f_2(t)$ for k_{uv} derivation (condition: 100 mg/L Cl_2, UVA irradiation, aerobic): $f_1 = \ln\frac{F}{F_0} + k_1 t; f_2 = \frac{([Cl_2]_0 - k_3 t)^2 - [Cl_2]_0^{\ 2}}{2k_3}$

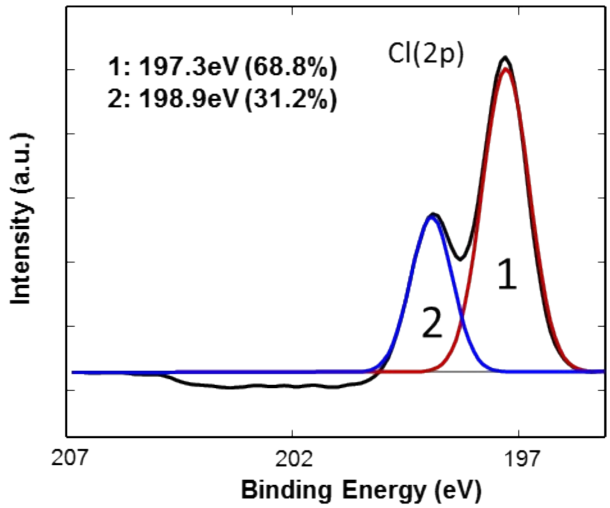

Fig. S3 Cl2p XPS spectrum of NaCl and curve fitting analysis**.**

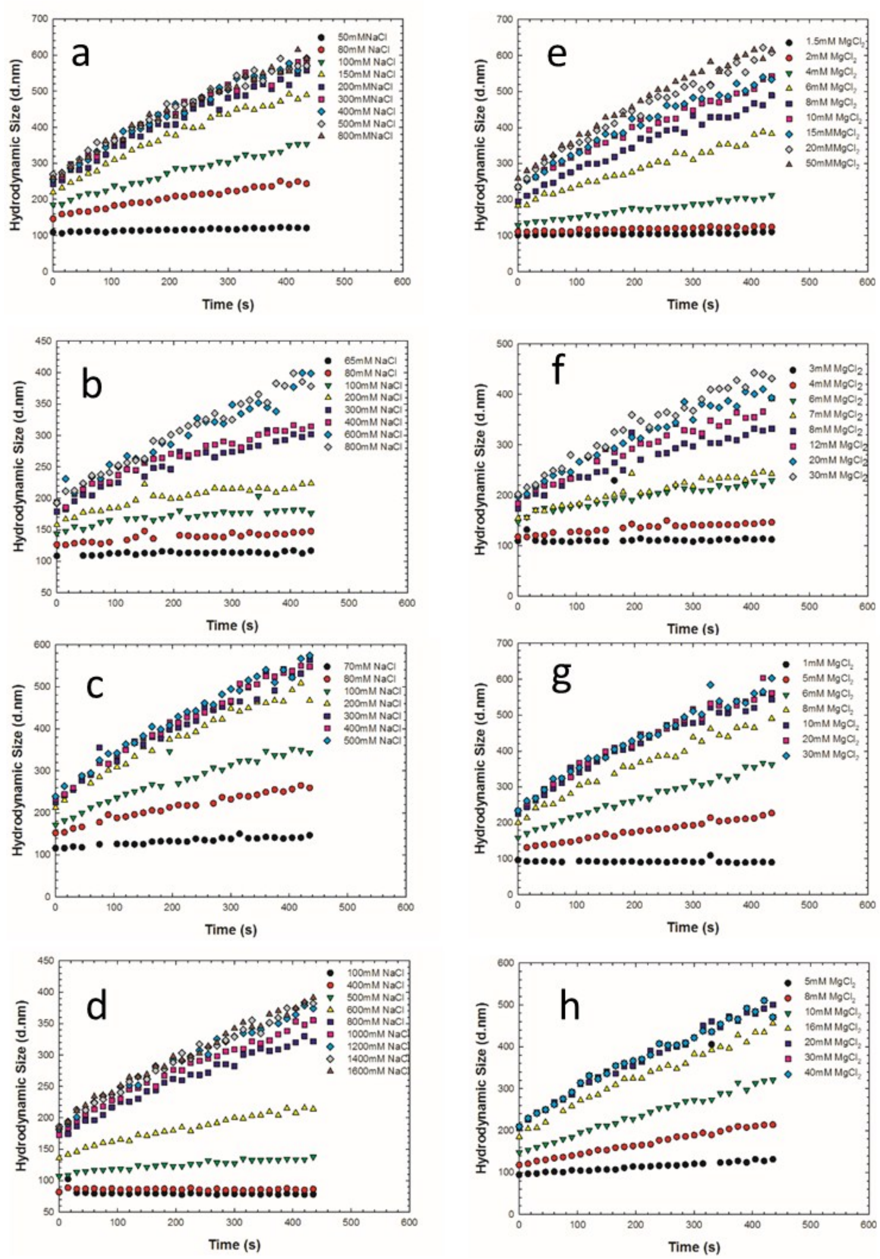

Fig. S4 Aggregation profiles of nC_{60} and reacted products in the presence of NaCl and $MgCl_2$ (pH ~ 6.5): (a) unreacted nC_{60} in NaCl; (b) reacted nC_{60} in dark (100mg/L Cl_2, 2h) in NaCl; (c) reacted nC_{60} under UV (no free chlorine, 2h) in NaCl; (d) reacted nC_{60} under UV (100 mg/L Cl_2, 2h) in NaCl; (e) unreacted nC_{60} in $MgCl_2$; (f) reacted nC_{60} in dark (100mg/L Cl_2, 2h) in $MgCl_2$; (g) reacted nC_{60} under UV (no free chlorine, 2h) in $MgCl_2$; (d) Reacted nC_{60} under UV (100 mg/L Cl_2, 2h) in $MgCl_2$.

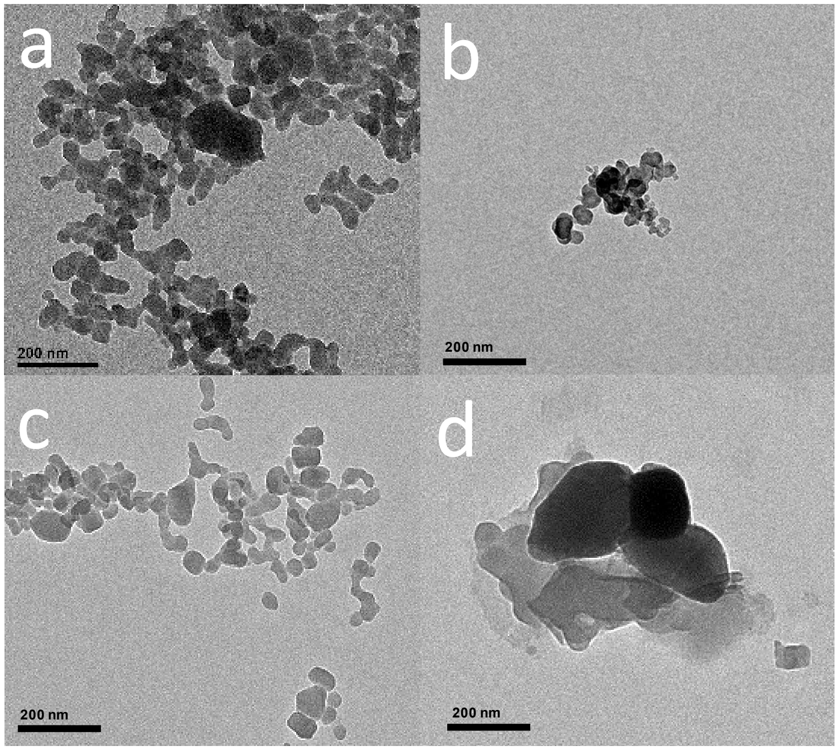

Fig. S5 TEM images of (a) Unreacted nC_{60}; (b) nC_{60} under UV irradiation for 2 hours; (c) nC_{60} with 100 mg/L Cl_2 in dark for 2 hours; (d) nC_{60} with 100 mg/L Cl_2 under UV for 2 hours. (Scale bar: 200 nm)

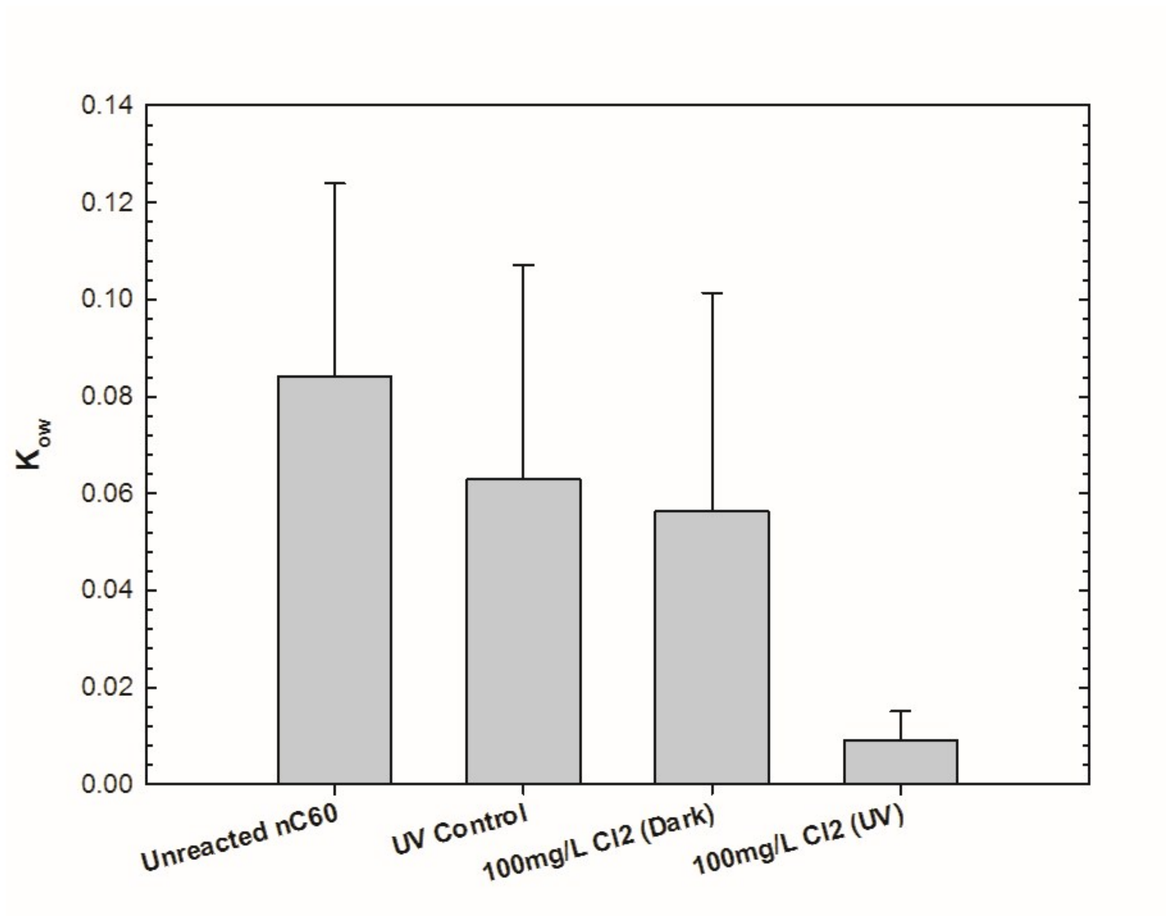

Fig. S6 Water-octanol coefficients (K_{ow}) of parent nC_{60} and reacted products under varied experimental conditions for 2 hours (pH ~ 7.5).

Table S1. C(1s) and Cl(2p) XPS analysis of nC_{60} and reacted products under varied experimental conditions.

C (1s)						Cl (2p)			
Peak 1		**Peak 2**		**Peak 3**		**Peak 1&2**		**Peak 3&4**	
Position (eV)	Ratio (%)	Position (eV)	Ratio (%)	Position (eV)	Ratio (%)	Position (eV)	Ratio (%)	Position (eV)	Ratio (%)
282.82	89.32	286.52	7.59	289.03	3.09	----	----	----	----
284.80	72.35	286.26	18.48	288.62	9.17	----	----	----	----
284.73	81.39	286.50	4.59	288.36	14.02	197.58/199.25	67.59/32.41	----	----
284.75	55.71	286.19	21.81	288.51	22.48	197.22/199.18	46.44/30.93	199.85/201.21	14.66/7.97

Reference

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