

Supplementary Information

Quantum confined Stark effect enabled non-intrinsic direct electron transfer for electrochemical water remediation

Jialong Yin ^{a,b}, Heng Zhang ^{a,b,*}, Mengfan Luo ^{a,b}, Zelin Wu ^{a,b}, Jia Zhao ^{a,b}, Tao Wei ^{a,b}, Bo Lai ^{a,b,c,*}

^a State Key Laboratory of Hydraulics and Mountain River Engineering, College of Architecture and Environment, Sichuan University, Chengdu 610065, China

^b Sino-German Centre for Water and Health Research, Sichuan University, Chengdu 610065, China

^c Key Laboratory of Jiangxi Province for Persistent Pollutants Prevention Control and Resource Reuse, Nanchang Hangkong University, Nanchang 330063, P. R. China

*Corresponding authors.

E-mail address: zhangheng01@scu.edu.cn (Heng Zhang); laibo@scu.edu.cn (Bo Lai);

Tel: +86 13008197875 (Heng Zhang); +86 19113174365 (Bo Lai)

15 **Supplementary Methods**

16 **Chemicals.** Glucose, sodium periodate (NaIO_4), sodium sulfate (Na_2SO_4), sodium thiosulfate
17 pentahydrate ($\text{Na}_2\text{S}_2\text{O}_3$), tert-Butanol (TBA), potassium dichromate ($\text{K}_2\text{Cr}_2\text{O}_7$), furfuryl alcohol
18 (FFA), *para*-benzopyrene (*p*-BQ), nitrotetrazolium blue chloride (NBT), tetramethylpiperidine
19 (TEMP), bisphenol A (BPA), phenol (PN), bisphenol F (BPF), 2,4-dichlorophenol (2,4-DCP), 4-
20 chlorophenol (4-CP), diclofenac (DCF), acetaminophen (ACT), sodium hydroxide (NaOH),
21 hydrochloric acid (H_2SO_4), were supplied by Aladdin Industrial Cooperation. All the above materials
22 utilized in this work are of analytical grade. Acetic acid, acetonitrile, methanol, and ammonium
23 formate with chromatographic grade were supplied by ANPEL Laboratory Technologies Inc.

24
25 **UHPLC-Q-TOF-MS/MS conditions.** The degradation intermediates of BPA were identified using
26 UHPLC-Q-TOF-MS/MS equipped with a BEH C18 column ($1.7\ \mu\text{m}$, $2.1 \times 50\ \text{mm}$) maintained at
27 $45\ ^\circ\text{C}$. Ammonium formate solution (0.1%, v/v) and methanol were used as mobile phases A and B,
28 respectively¹. The gradient elution program was as follows: 5% B for the initial 3 min, increased
29 linearly to 50% B at 7 min, then to 95% B at 8 min and held for 4 min. Subsequently, the mobile
30 phase was returned to 5% B within 1 min and equilibrated for 2 min. Mass spectra were acquired in
31 the negative electrospray ionization (ESI[−]) mode over an m/z range of 20–1000.

32
33 **Electrochemical measurements.** Electrochemical measurements were conducted using a
34 conventional three-electrode system controlled by a CHI 760E electrochemical workstation. A
35 platinum wire served as the counter electrode, and a saturated calomel electrode (SCE) was used as
36 the reference electrode. The electrolyte consisted of a 50 mM Na_2SO_4 aqueous solution maintained

37 at ambient temperature. For CV experiments, the NF electrode (1 cm × 1 cm) was employed as the
38 working electrode, while OCV measurements utilized a glassy carbon (GC) electrode.

39 Electrode capacitance characterization involved performing CV scans at scan rates ranging from
40 20 to 100 mV s⁻¹ within the non-faradaic potential window (from 0.0 V to 0.6 V vs. SCE) with
41 incremental additions of carbon quantum dots (CQDs). The electrode capacitance was determined by
42 plotting the average current difference at the current window against the scan rate and calculating the
43 linear regression slope. Faraday current tests of PI and CQDs-PI complexes employed CV scans over
44 a faradaic potential range (from -0.5 V to 1.5 V vs. SCE) at 50 mV s⁻¹. Key redox features (peak
45 potentials, currents) were extracted from the first cycle. OCV analysis under applied potential
46 integrated the three-electrode system into a CQDs three-dimensional electrode reactor, monitoring
47 OCV evolution at fixed reactor potentials until stabilization.

48
49 **Density functional theory (DFT) calculations.** DFT calculations were performed using the
50 Gaussian 16 software package. Ground-state geometry optimizations and frequency calculations
51 employed the hybrid B3LYP exchange-correlation functional with a mixed basis set: the 6-311G basis
52 set for C, H, and O atoms, and the def2-TZVP effective core potential and basis set for the I atom.
53 Solvent effects (water) were incorporated using the SMD continuum solvation model. Grimme's D3
54 dispersion correction with Becke-Johnson damping (GD3BJ) was applied to all calculations to
55 account for van der Waals interactions. For calculations under an applied external electric field, the
56 molecular Cartesian coordinate system was aligned to ensure the field vector was precisely anti-
57 parallel to the molecular dipole moment vector, the magnitude of the electric field intensity is set at
58 the order of 10⁻⁶ a.u., which is in line with the range of the actual applied electric field. Singlet excited

states of CQDs were calculated using time-dependent DFT (TDDFT) within the linear response framework, employing the PBE functional. The lowest five singlet excitations were computed, and the lowest-energy singlet excitation (S_1) was analyzed. The linear response (LR) solvent model within the SMD framework was utilized for TDDFT calculations to accurately describe solvatochromic shifts. All calculations employed tight convergence criteria for both the self-consistent field (SCF) cycles and geometry optimizations.

COMSOL simulations. Multiphysics simulations were performed using COMSOL Multiphysics software (version 6.3). A 3D geometric model of the reactor was constructed based on its actual dimensions and material properties. The electrostatic field distribution was computed using the electrostatics interface. A voltage difference was applied between the two electrode plates to replicate the experimental electric field configuration, and the steady-state potential distribution was solved via a stationary study. Subsequently, PI concentration distribution was modeled by coupling the predefined electric field to the transport of diluted species interface. The initial PI concentration was set to 1.5 mM with a charge number of -1 . The transient diffusion-electromigration process was simulated over a 2-second duration using a time-dependent study. The electric currents and transport of diluted species interfaces were bidirectionally coupled to capture the interplay between ion migration and field evolution. Mesh independence was verified through convergence tests, and solver tolerances were tightened to ensure numerical accuracy ($\pm 0.5\%$ relative error).

Pseudo-first-order kinetics. The pollutant removal of E-CQDs/PI and other systems followed the pseudo-first-order kinetics. The apparent reaction rate constants (k_{obs} , min^{-1}) were obtained via eq.

81 S1.

$$82 \quad k_{\text{obs}} = \frac{-\ln\left(\frac{C_t}{C_0}\right)}{t} \quad (S1)$$

83 Where C_0 (μM) and C_t (μM) are the concentrations of BPA at the initial time and at time t (min).

84

85 **NBT probe for $\text{O}_2^{\bullet-}$ Identification.** Nitroblue tetrazolium dichloride (NBT) could be utilized to
86 determine the generation of $\text{O}_2^{\bullet-}$ since $\text{O}_2^{\bullet-}$ could attack ditetrazolium (NBT^{2+}) to generate tetrazolyl
87 radical ($\text{NBT}^{\bullet+}$). Then $\text{NBT}^{\bullet+}$ rapidly transferred to purple formazan that could be measured with
88 maximum absorbance at 560 nm^2 .

89 For measurement, 0.1 mM NBT was added to the sample before treatment, after 20 min
90 treatment, 1 mL sample was collected to add to 3 mL ultrapure water for subsequent UV-vis analysis.

91

92 **Acid-base titration experiment.** To conduct the titration experiment, 0.08 g of NaOH was dissolved
93 in 20 mL of CQDs solution (10 g/L). After stirring for 2 hours , 10 mL of the alkaline-treated solution
94 was withdrawn and diluted to 50 mL with pure water. Then, the diluted solution was titrated with 0.1
95 M HCl. Ultrapure water solution was used as the control group for the experiment. The difference in
96 the volumes of HCl in the two titration curves for the same value of pH gave the concentration of the
97 ionized groups of CQDs at that pH³.

98 For the detection of the surface functional group concentration of the CQDs-PI complex, 100
99 mL of CQDs solution was replaced with a mixed solution of CQDs and PI (50 mL of 20 g/L CQDs
100 and 50 mL of 25 mM PI). The remaining steps were the same as those for the determination of the
101 CQDs solution.

102

103 **PI products analysis.** The products of the PI reaction, including hypiodite (HOI) and iodine (I₂),
104 were investigated⁴. The detection of HOI was achieved through a characteristic product method,
105 utilizing phenol as a trapping agent. HOI reacts with phenol to yield 4-iodophenol (4-IP) and 2-
106 iodophenol (2-IP), which were subsequently analyzed using HPLC. The detection of I₂ was conducted
107 via a starch colorimetric method. 3 g stock solution of soluble starch was prepared by dissolving it in
108 10 mL of deionized water, followed by the addition of 90 mL of boiling water while stirring
109 magnetically for 10 minutes. The mixture was then cooled to room temperature to obtain the starch
110 stock solution. The reaction mixture from the E-CQDs/PI system under both conditions, along with
111 a 0.75 mM iodine standard solution, was mixed with the starch stock solution. The
112 resulting solution turned blue, indicating the presence of I₂ within the system.

113

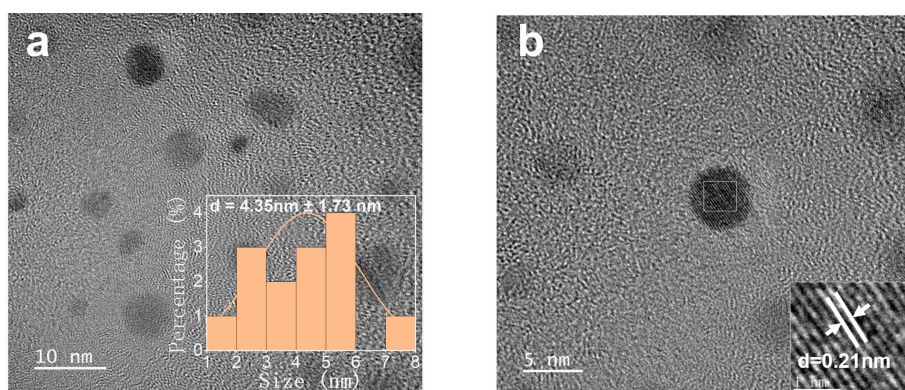
114 **Calculation of the electric energy per order (E_{EO}).** E_{EO} (kWh m⁻³ order⁻¹) is the amount of
115 electrical energy required to reduce a contaminant by one order of magnitude in the range of one
116 cubic meter, which is calculated by eq. S2.

117
$$E_{EO} = \frac{1000Pt}{60V \lg(\frac{C_0}{C_t})} = \frac{38.4 \times P}{V \times k_{obs}} \quad (S2)$$

118 Where P is the total electrical power (kW), t is the reaction time (min), V is the solution volume
119 (L), C₀ and C_t are the concentrations of BPA at the initial time and at time t (μM), k_{obs} is the first-
120 order rate constant for BPA removal (min⁻¹).

121

122 **Supplementary Figures**

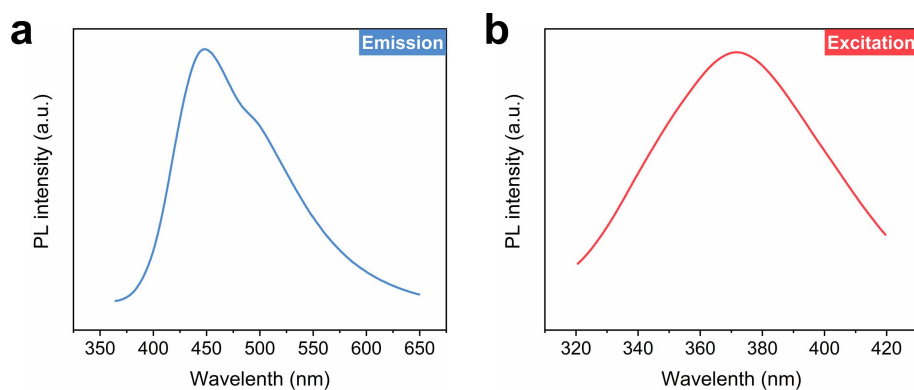


123

124 **Supplementary Fig. 1. a,b**, TEM image of CQDs (scale bar: 10 nm), with the inset showing the size
125 distribution (a). High-resolution TEM image of CQDs (scale bar: 5 nm), with the inset showing the
126 lattice spacing (b).

127 TEM images showed that CQDs were spherical nanoparticles with an average diameter of 4.35
128 nm (**Supplementary Fig. 1a**). HRTEM analysis revealed clear lattice fringes with a spacing of 0.21
129 nm, assigned to the (100) plane of graphitic carbon (**Supplementary Fig. 1b**).

130

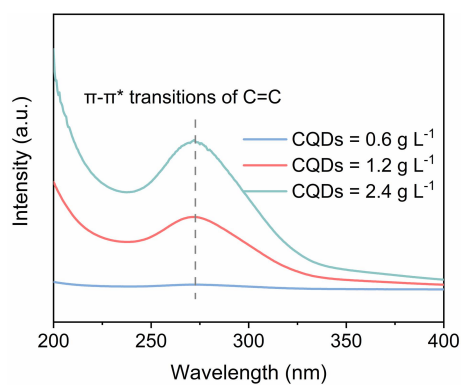


131

132 **Supplementary Fig. 2. a,b,** Photoluminescence (PL) spectra of CQDs, including **(a)** emission and
 133 **(b)** excitation spectra.

134 The PL spectra of CQDs exhibited prominent emission and excitation peaks centered at 440 and
 135 370 nm, respectively. The strong PL intensity reflects the intrinsic photoluminescence capability of
 136 CQDs, suggesting their favorable electronic properties and well-defined surface states.

137

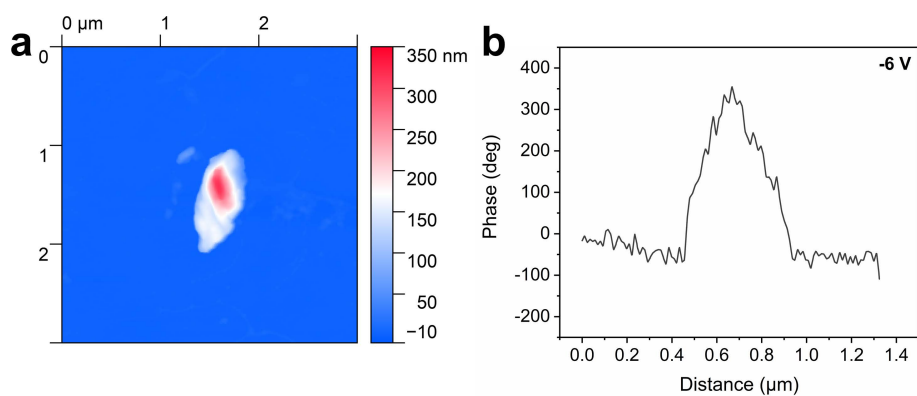


138

139 **Supplementary Fig. 3.** UV-vis spectrum of CQDs.

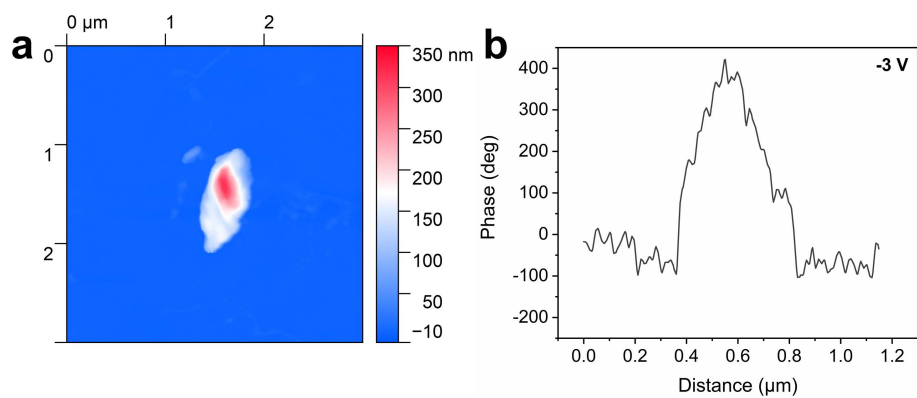
140 The UV-vis absorption spectrum of CQDs exhibited a prominent peak at 275 nm, which can be
 141 assigned to the π - π transition of sp^2 C=C bonds. This characteristic feature indicates the presence of
 142 abundant conjugated carbon structures within the CQDs, suggesting the formation of graphitic
 143 domains and extended π -electron systems.

144



145

146 **Supplementary Fig. 4. a,b**, AFM image of selected CQDs (**a**). Corresponding spatial distribution of
 147 the EFM phase signal on the CQDs surface under an applied tip voltage of -6 V (**b**).
 148

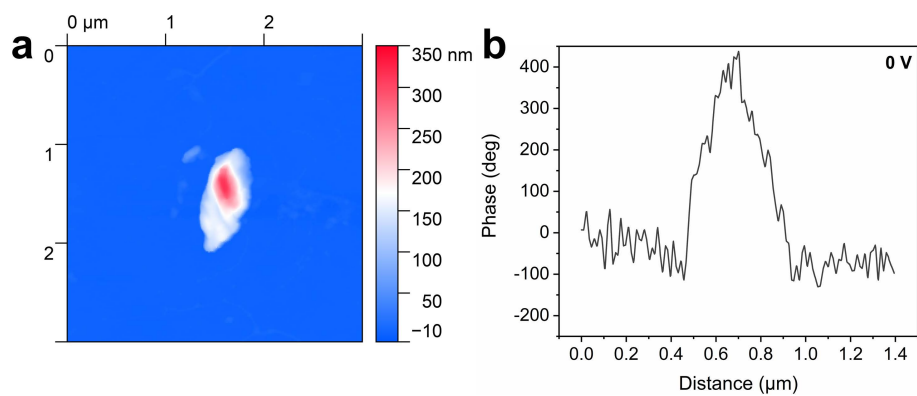


149

150 **Supplementary Fig. 5. a,b**, AFM image of selected CQDs (**a**). Corresponding spatial distribution of

151 the EFM phase signal on the CQDs surface under an applied tip voltage of -3 V (**b**).

152

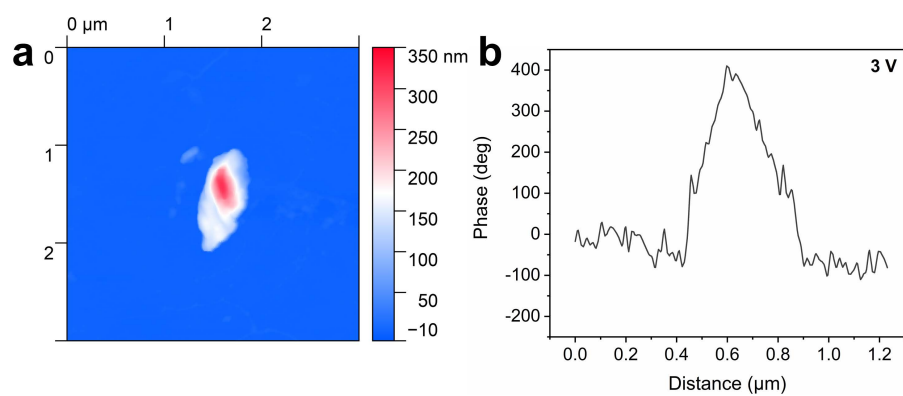


153

154 **Supplementary Fig. 6. a,b**, AFM image of selected CQDs (**a**). Corresponding spatial distribution of

155 the EFM phase signal on the CQDs surface without tip voltage application (**b**).

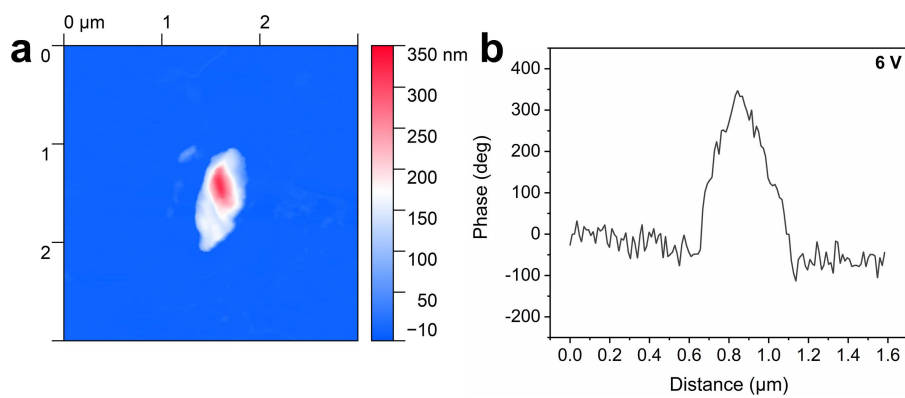
156



157

158 **Supplementary Fig. 7. a,b**, AFM image of selected CQDs (a). Corresponding spatial distribution of
 159 the EFM phase signal on the CQDs surface under an applied tip voltage of 3 V (b).

160

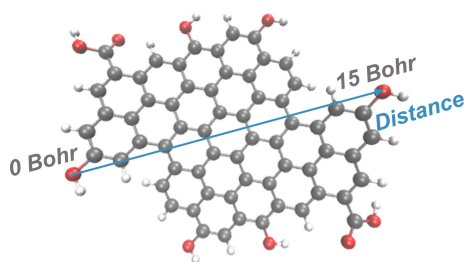


161

162 **Supplementary Fig. 8. a,b**, AFM image of selected CQDs (**a**). Corresponding spatial distribution of

163 the EFM phase signal on the CQDs surface under an applied tip voltage of 6 V (**b**).

164

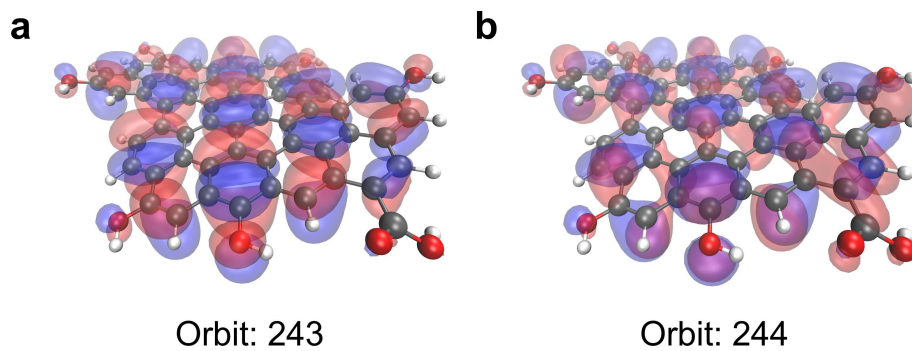


165

166 **Supplementary Fig. 9.** Schematic diagram of the calculated line on the CQDs aligns with the dipole

167 direction.

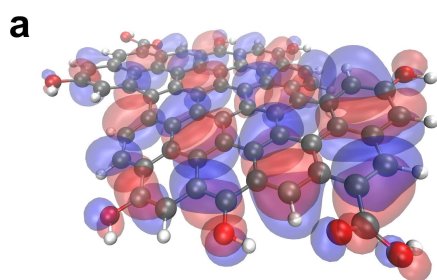
168



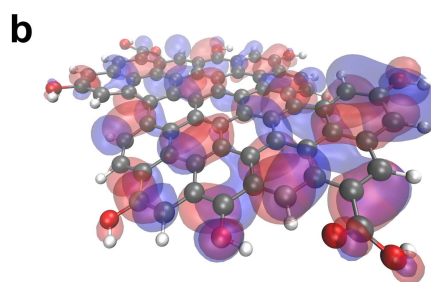
169

170 **Supplementary Fig. 10. a,b**, 243 (a) and 244 (b) excitation orbits of CQDs without the external
171 electric field.

172



Orbit: 243



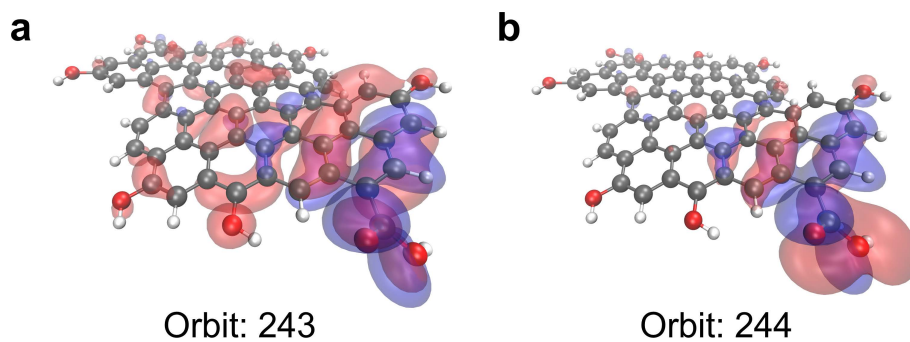
Orbit: 244

173

174 **Supplementary Fig. 11. a,b, 243 (a) and 244 (b) excitation orbits of CQDs with the external electric**

175 field intensity of 1.25×10^{-6} a.u..

176

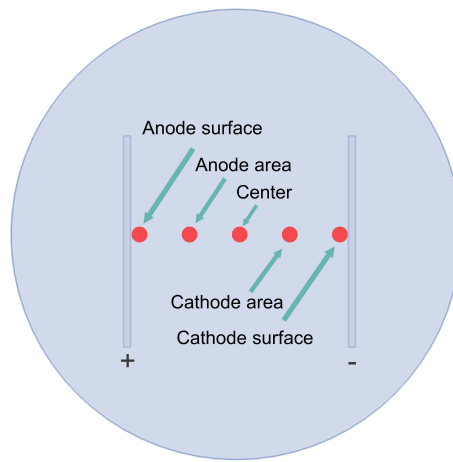


177

178 **Supplementary Fig. 12. a,b, 243 (a) and 244 (b) excitation orbits of CQDs with the external electric**

179 field intensity of 2.0×10^{-6} a.u..

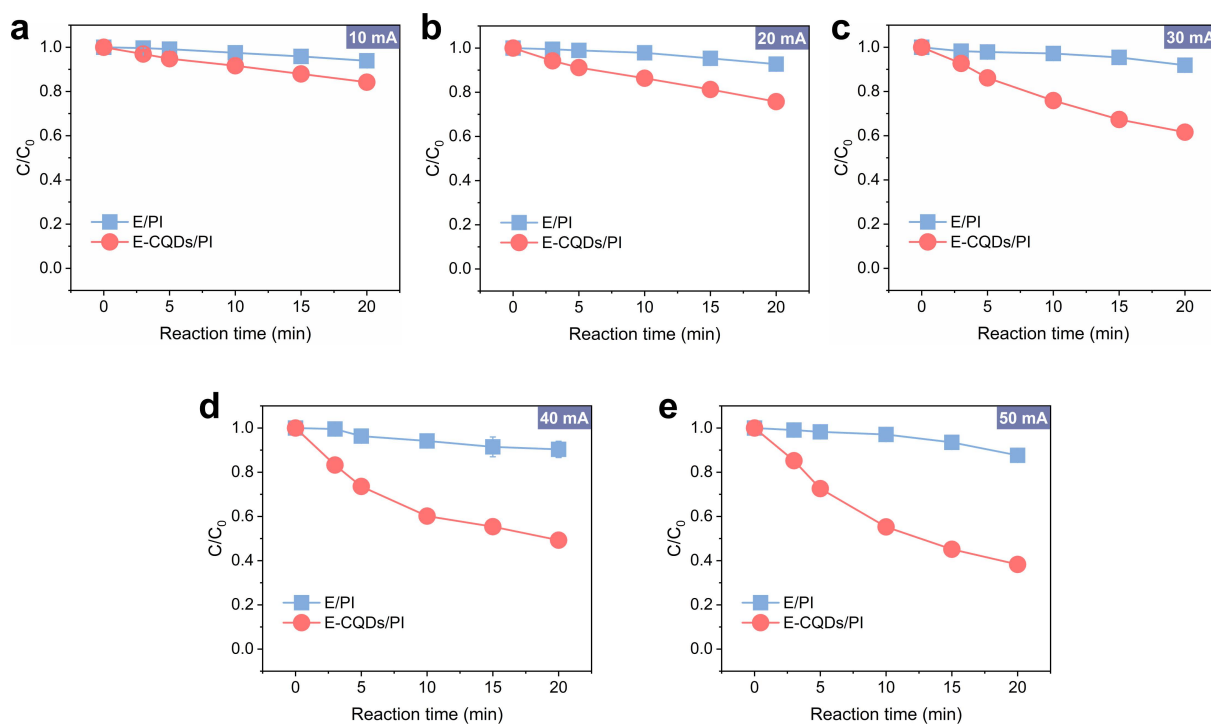
180



181

182 **Supplementary Fig. 13.** The diagrammatic drawing of five positions in the OCP test.

183



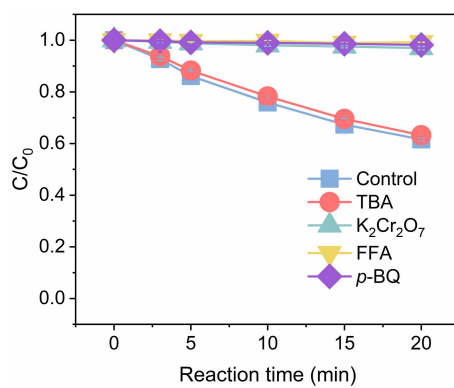
184

185 **Supplementary Fig. 14. a-e**, BPA removal performance of the E/PI and E-CQDs systems under

186 various anodic current intensities. (a) 10 mA; (b) 20 mA; (c) 30 mA; (d) 40 mA; (e) 50 mA.

187 Experimental conditions: [CQDs] = 1.2 g L⁻¹, [PI] = 1.5 mM, [BPA] = 20 μM.

188

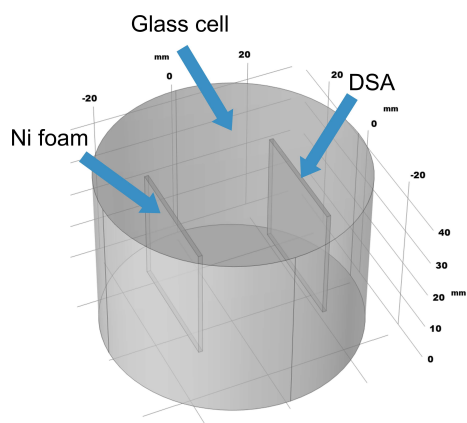


189

190 **Supplementary Fig. 15.** Removal rate of BPA with the addition of various scavengers. Experimental

191 conditions: [TBA] = [FFA] = [L-HIS] = [p-BQ] = 100 mM.

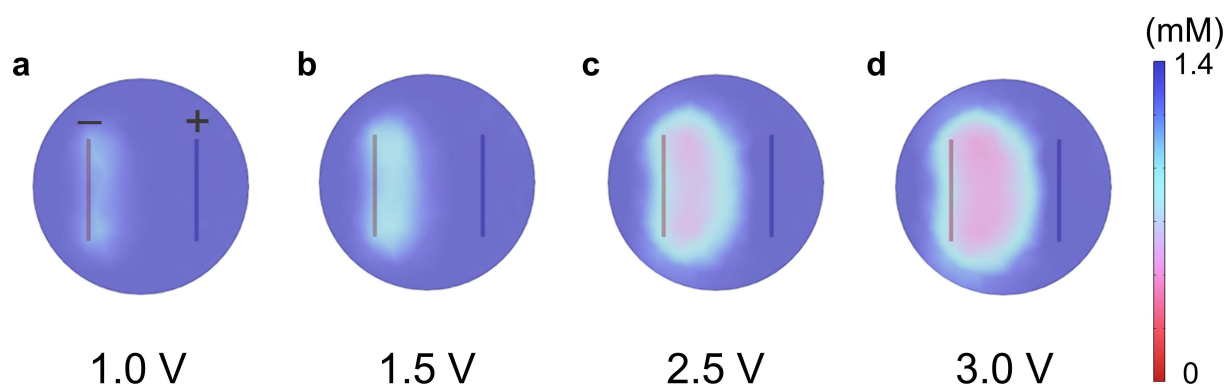
192



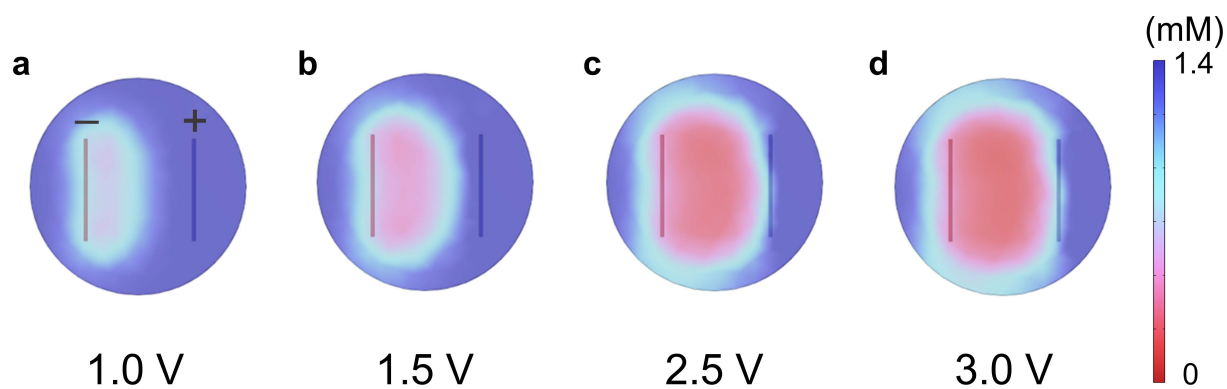
193

194 **Supplementary Fig. 16.** Model of the reaction device for the E-CQDs/PI system.

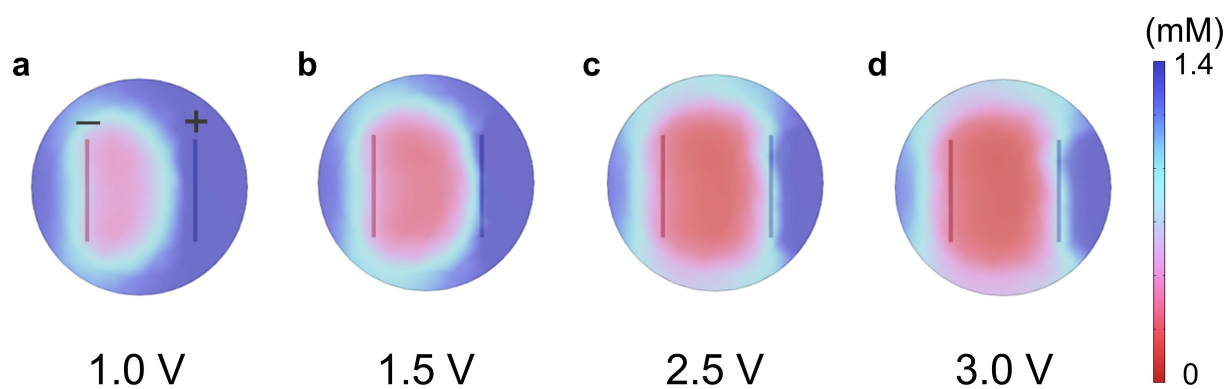
195



Supplementary Fig. 17. a-d, Simulated PI concentration distributions in the reactor at 0.5 s under different applied voltages: **(a)** 1.0 V, **(b)** 1.5 V, **(c)** 2.5 V, and **(d)** 3.0 V. (The cathode and anode are located on the left and right sides, respectively).



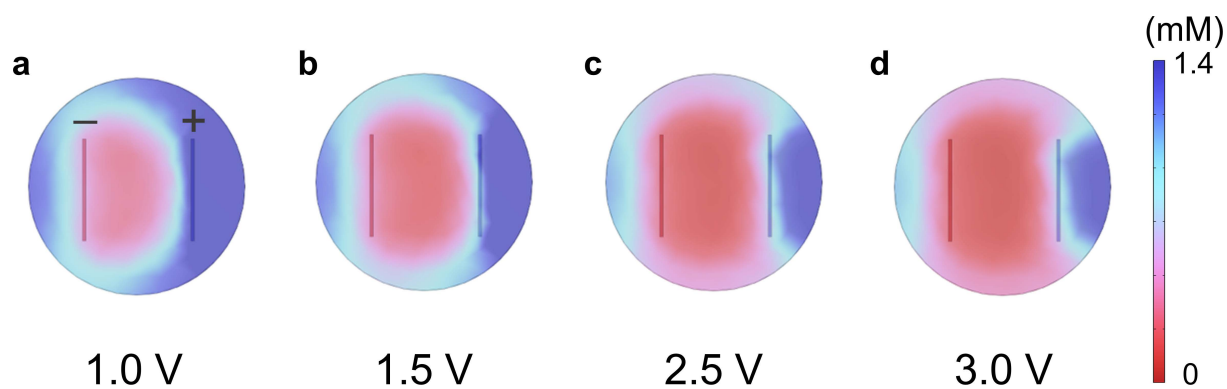
Supplementary Fig. 18. a-d, Simulated PI concentration distributions in the reactor at 1.0 s under different applied voltages: **(a)** 1.0 V, **(b)** 1.5 V, **(c)** 2.5 V, and **(d)** 3.0 V. (The cathode and anode are located on the left and right sides, respectively).



206

207 **Supplementary Fig. 19. a-d**, Simulated PI concentration distributions in the reactor at 1.5 s under
 208 different applied voltages: **(a)** 1.0 V, **(b)** 1.5 V, **(c)** 2.5 V, and **(d)** 3.0 V. (The cathode and anode are
 209 located on the left and right sides, respectively).

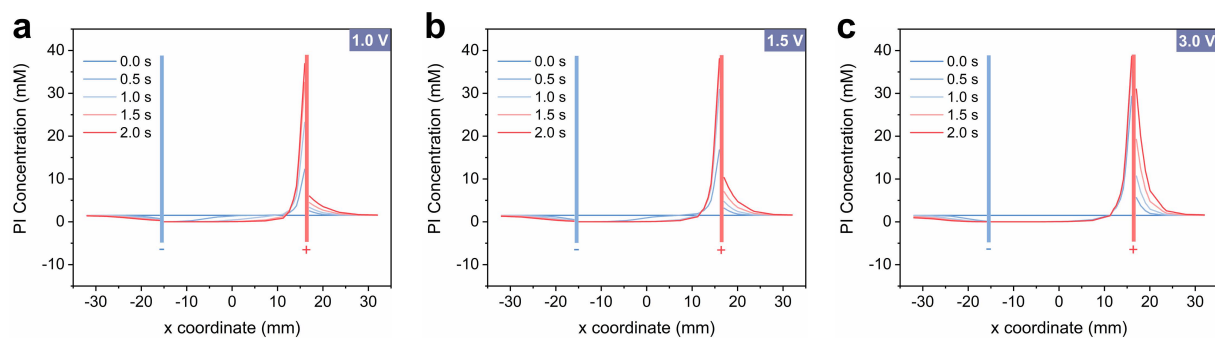
210



211

212 **Supplementary Fig. 20. a-d**, Simulated PI concentration distributions in the reactor at 2.0 s under
 213 different applied voltages: **(a)** 1.0 V, **(b)** 1.5 V, **(c)** 2.5 V, and **(d)** 3.0 V. (The cathode and anode are
 214 located on the left and right sides, respectively).

215

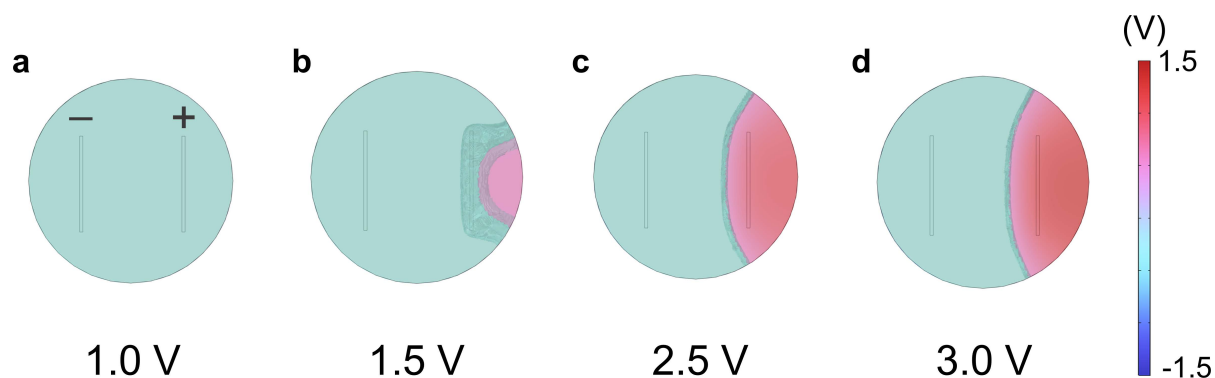


216

217 **Supplementary Fig. 21. a-c**, Simulated PI concentration distribution along the x-axis at an applied

218 voltage of 1.0 V (a), 1.5 V (b), and 3.0 V (c).

219

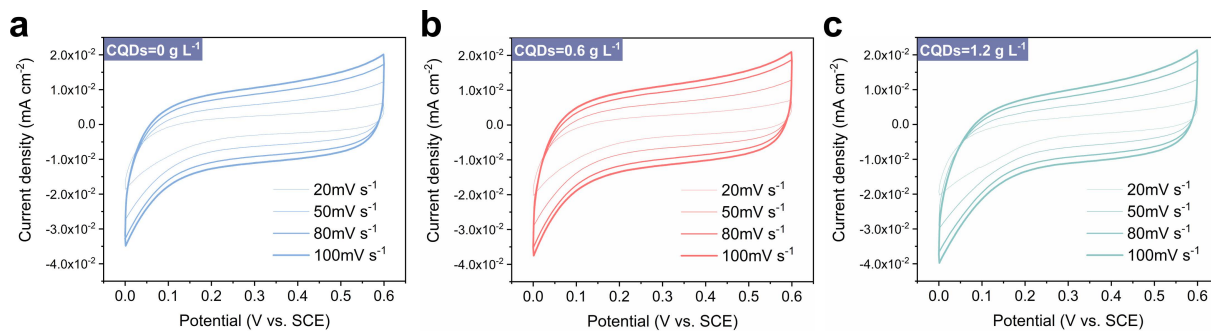


220

221 **Supplementary Fig. 22.** a-d, Simulated electric potential distributions within the device under
 222 different applied voltages: (a) 1.0 V, (b) 1.5 V, (c) 2.5 V, and (d) 3.0 V, together with the corresponding
 223 spatial distributions of PI activation regions (The cathode and anode are located on the left and right
 224 sides, respectively).

225 The cyan colors represent the activation areas of PI, which were derived from the results of CV
 226 tests within the Faraday range (0.12 to 0.62 V vs. SCE) (**Fig. 4e**).

227

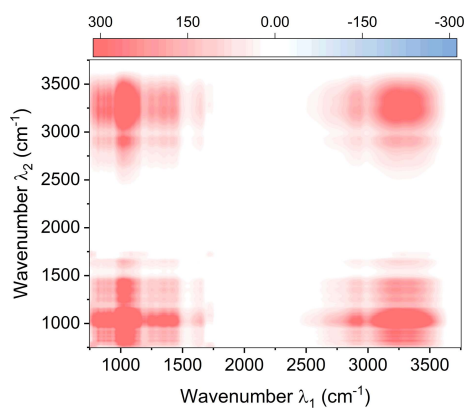


228

229 **Supplementary Fig. 23. a-c**, The CV curves of the non-Faraday region were measured at 0 g/L (a),

230 0.6 g/L (b), and 1.2 g/L (c) of CQDs.

231

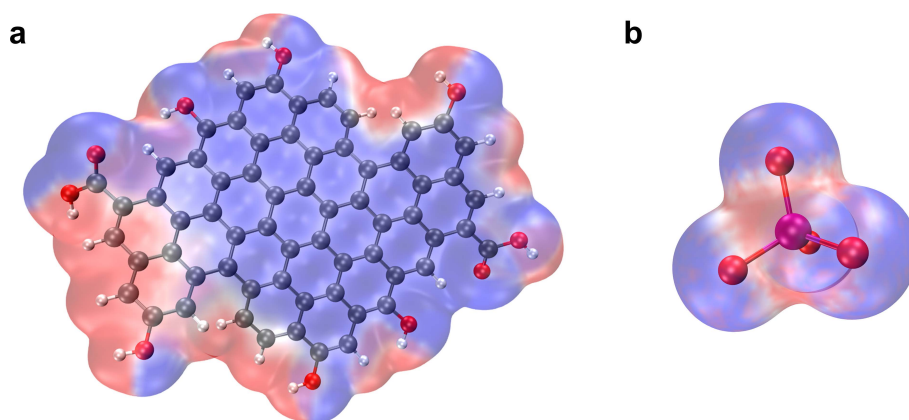


232

233 **Supplementary Fig. 24.** Synchronous 2D-COS maps generated from the FTIR spectra of CQDs-PI

234 complexes.

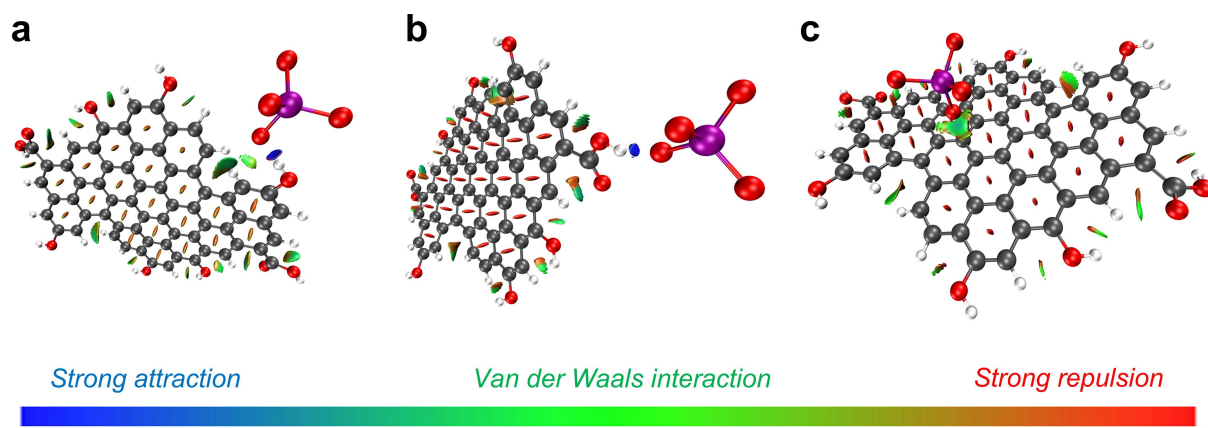
235



236

237 **Supplementary Fig. 25. a,b,** The ESP distribution of CQDs (**a**) and PI (**b**) (The blue and red areas
 238 represent electron-rich and electron-deficient regions, respectively).

239

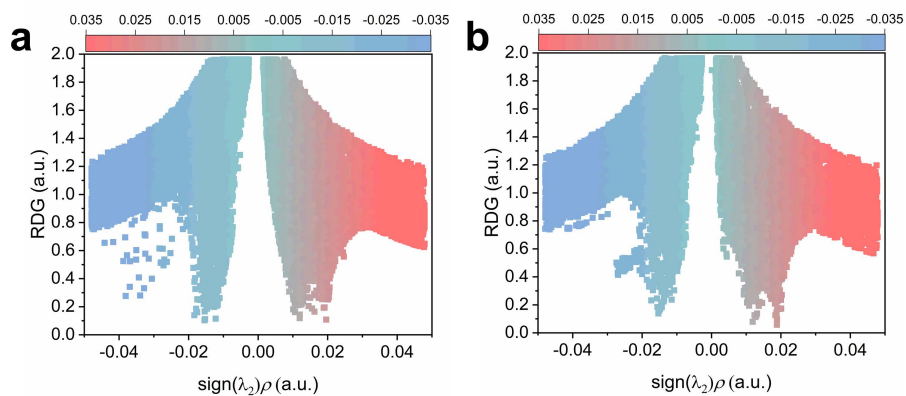


240

241 **Supplementary Fig. 26. a-c**, The intensity of weak interaction adsorption between PI and CQDs via

242 -OH (a), -COOH (b), and carbon base (c).

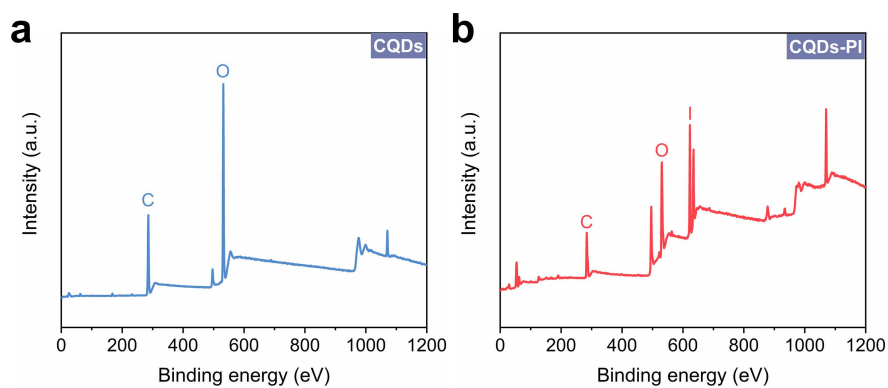
243



244

245 **Supplementary Fig. 27. a,b**, Corresponding plots of the RDG versus the electron density (ρ)
 246 multiplied by the sign of the second Hessian eigenvalue (λ_2). **(a)** $-\text{COOH}$ of CQDs; **(b)** carbon base
 247 of CQDs.

248

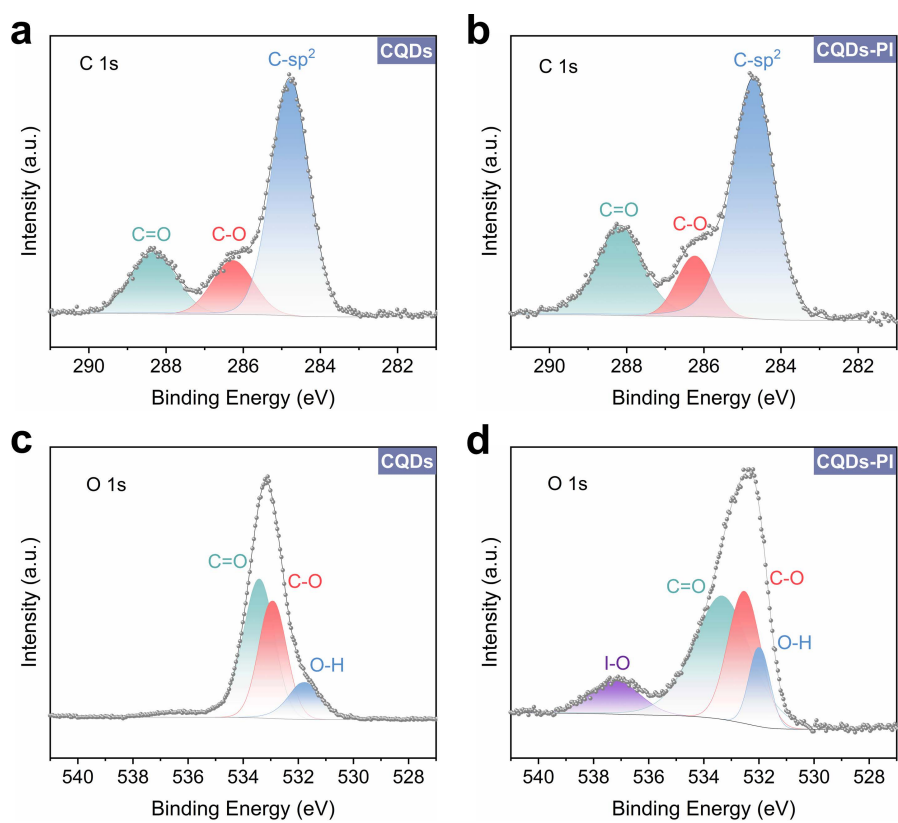


249

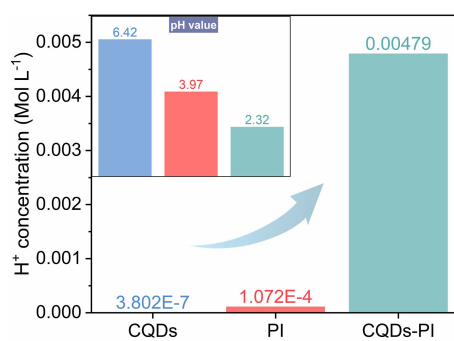
250 **Supplementary Fig. 28. a,b**, Types of surface elements of CQDs before (a) and after (b) PI

251 adsorption.

252



Supplementary Fig. 29. a-d, XPS spectrum of CQDs and CQDs-PI, C 1s (a, b), and O 1s (c, d).

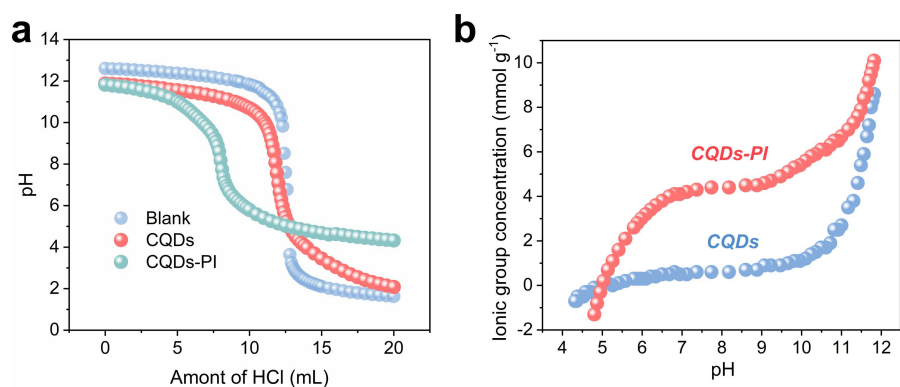


256

257 **Supplementary Fig. 30.** Proton concentration of CQDs, PI, and CQDs-PI solutions (The insert image

258 shows the pH value of these systems).

259

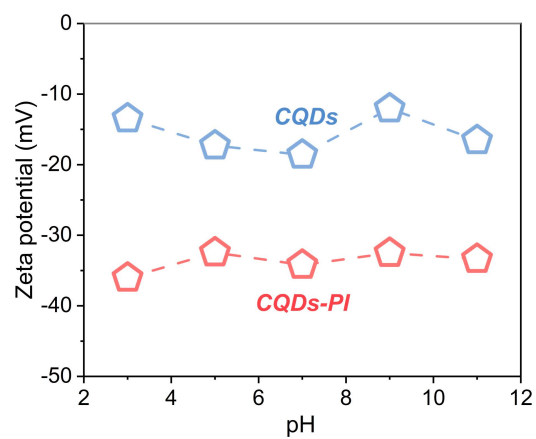


260

261 **Supplementary Fig. 31. a,b,** The pH titration curves of blank, CQDs, and CQDs-PI solutions (**a**).

262 The ionic group concentration of CQDs and CQDs-PI solutions (**b**).

263

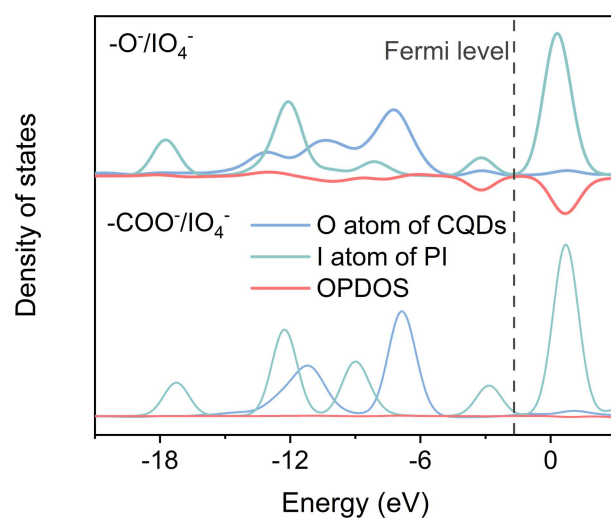


264

265 **Supplementary Fig. 32.** Zeta potential of CQDs and CQDs-PI solutions at various pH conditions.

266 The DOS of the O and I atom orbital with O^- and COO^- adsorption and their OPDOS.

267

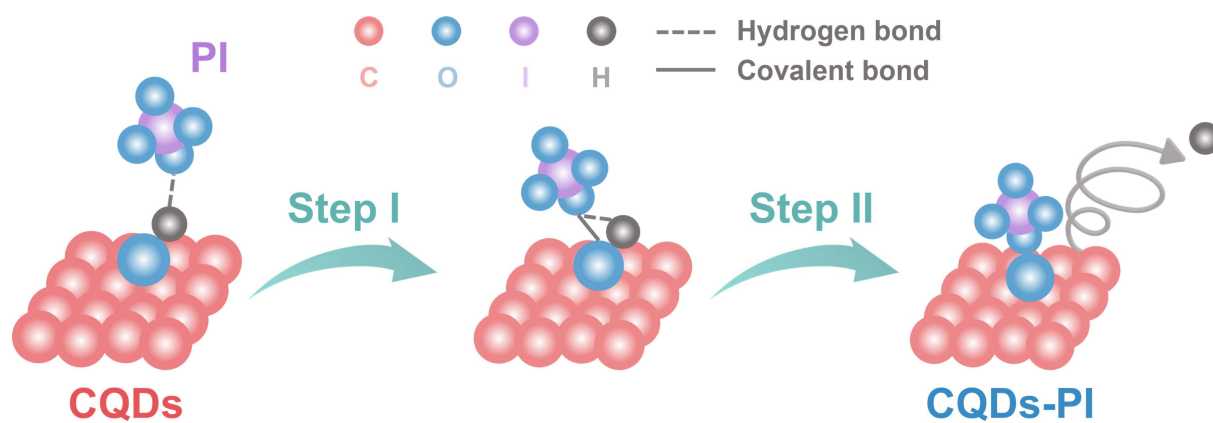


268

269 **Supplementary Fig. 33.** The DOS of the O and I atom orbital with $-O^-$ and $-COO^-$ adsorption and

270 their OPDOS.

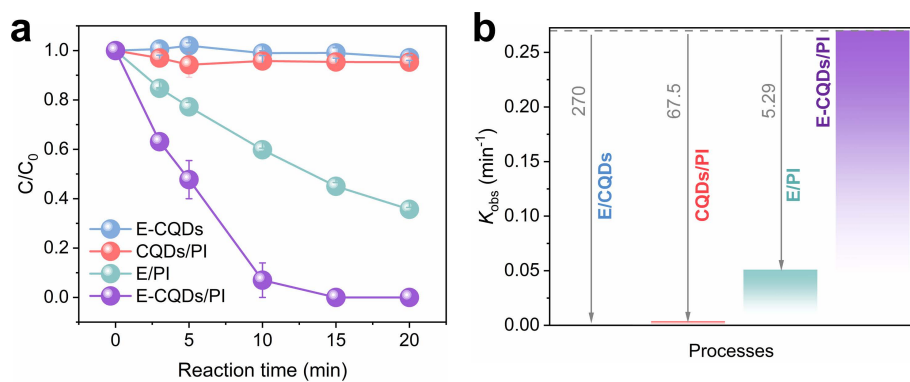
271



272

273 **Supplementary Fig. 34.** Schematic diagram of CQDs adsorbing PI.

274



275

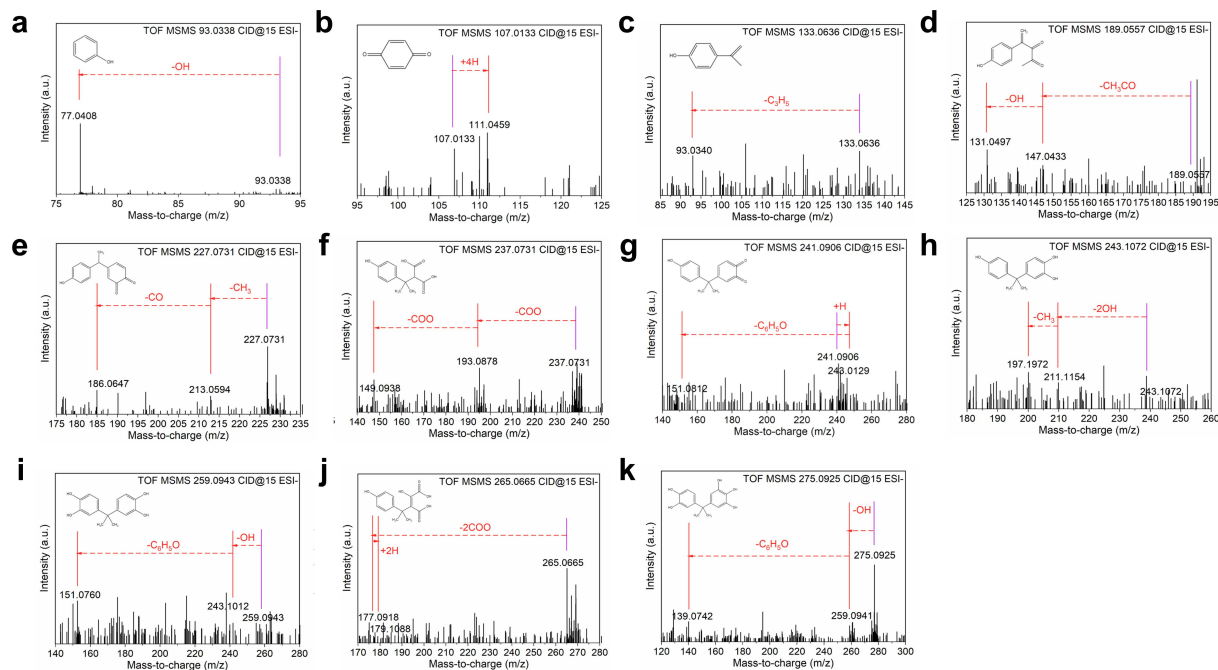
276 **Supplementary Fig. 35. a,b**, BPA removal efficiency (a) and corresponding kinetics (b) of different

277 systems in the single-cell device. Experimental conditions: [CQDs] = 1.2 g L⁻¹, [PI] = 1.5 mM, [BPA]

278 = 20 μM, applied current = 30 mA.

279

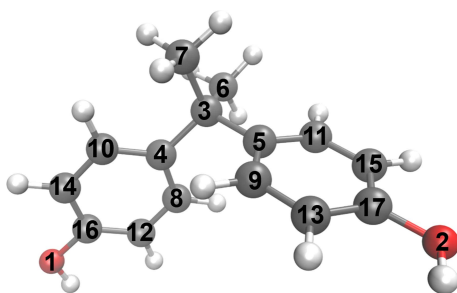
280



281

Supplementary Fig. 36. a-k, Mass structure and proposed fragment structure for BPA degradation intermediates. (a) TP-93; (b) TP-107; (c) TP-133; (d) TP-189; (e) TP-227; (f) TP-237; (g) TP-241; (h) TP-243; (i) TP-259; (j) TP-265; (k) TP-275.

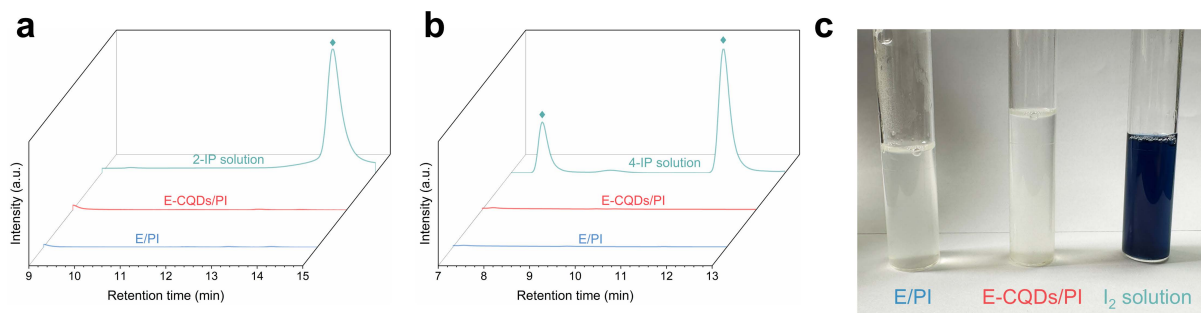
285



286

287 **Supplementary Fig. 37.** The atomic number of BPA used in the calculation of the Fukui index.

288



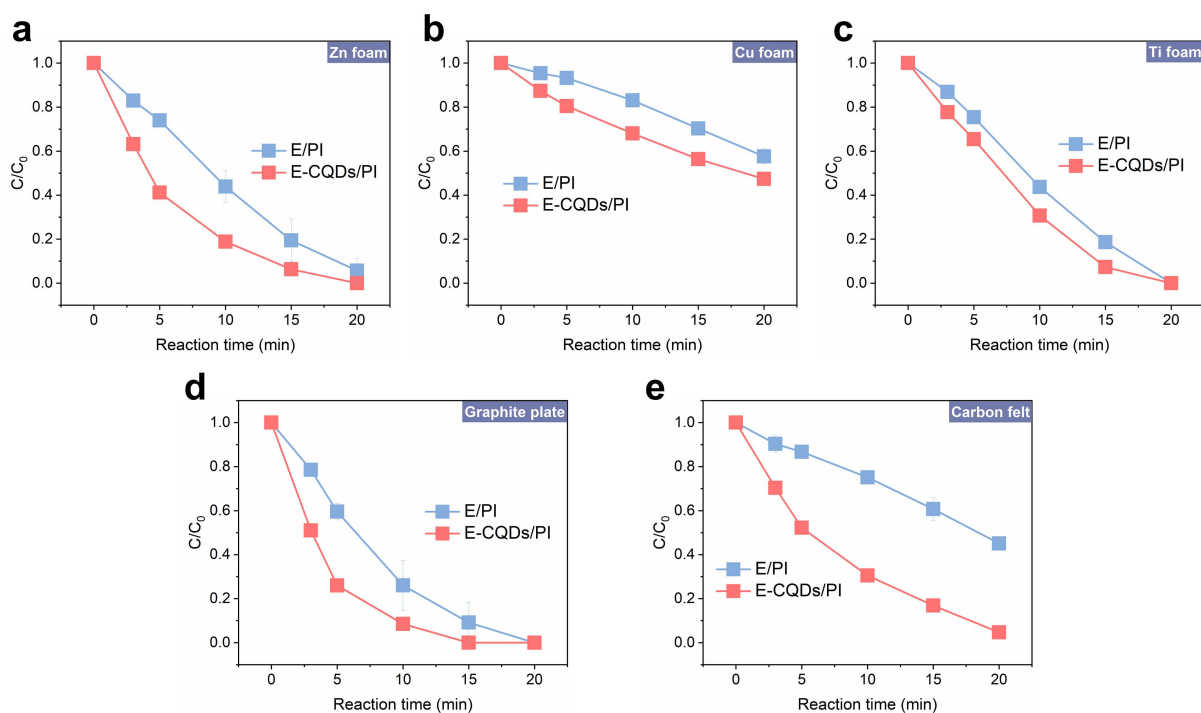
289

290 **Supplementary Fig. 38. a-c**, Liquid chromatogram spectra of 2-IP (**a**) and 4-IP (**b**), and starch

291 colorimetry of I₂ (**c**) in the E-CQDs/PI system. Experimental conditions: [2-IP] = [4-IP] = 1.5 mM,

292 [I₂] = 0.75 mM.

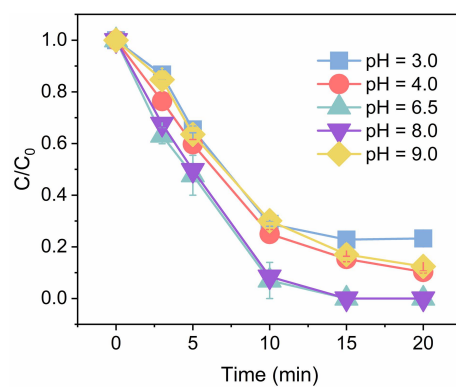
293



294

295 **Supplementary Fig. 39. a-e**, The efficiency of E/PI and E-CQDs/PI systems in removing BPA for
 296 different cathode materials. **(a)** Zn foam; **(b)** Cu foam; **(c)** Ti foam; **(d)** Graphite plate; **(e)** Carbon
 297 felt.

298

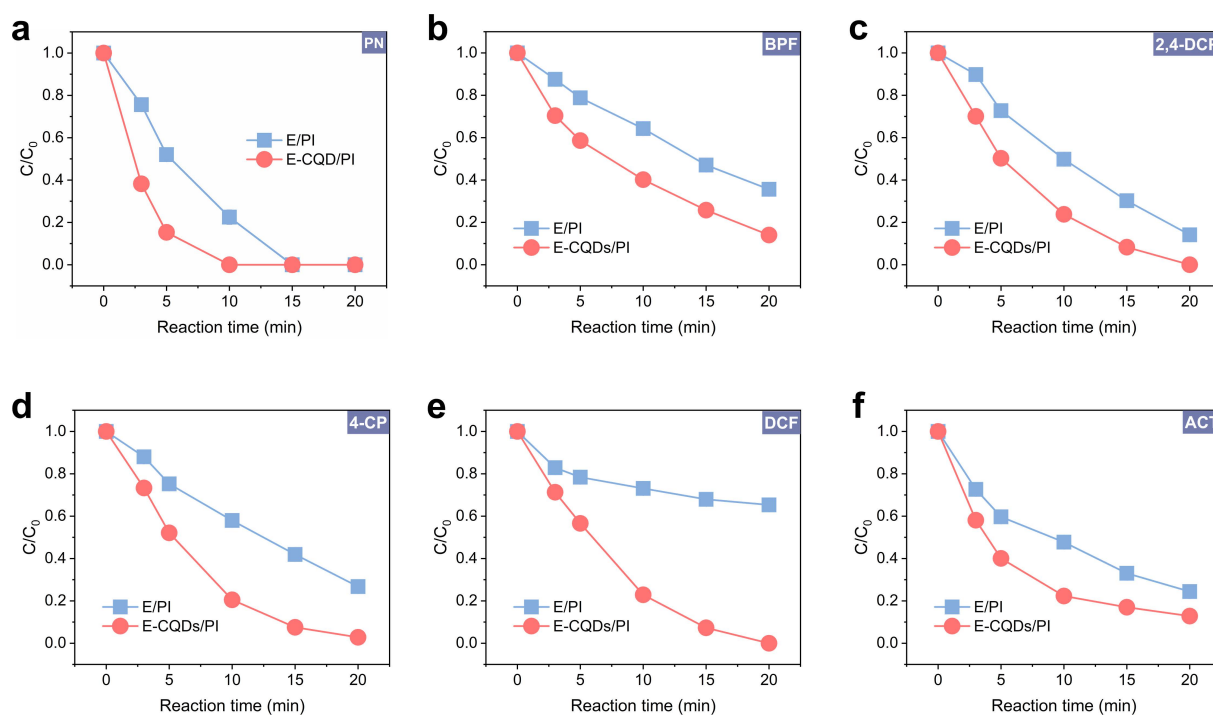


299

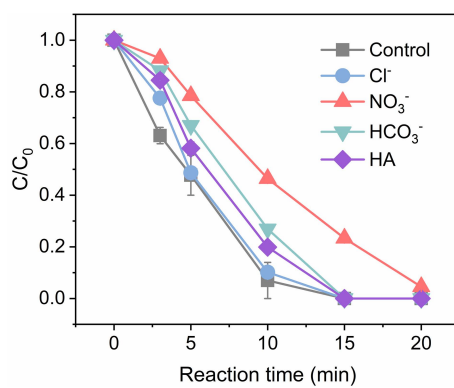
300 **Supplementary Fig. 40.** The BPA degradation efficiency of the E-CQDs/PI system in different pH

301 conditions.

302



Supplementary Fig. 41. a-f, The efficiency of E/PI and E-CQDs/PI systems in removing different pollutants. **(a)** phenol (PN); **(b)** bisphenol F (BPF); **(c)** 2,4-dichlorophenol (2,4-DCP); **(d)** 4-chlorophenol (4-CP); **(e)** diclofenac (DCF); **(f)** acetaminophen (ACT). Experimental conditions: [PN] = [BPF] = [2,4-DCP] = [4-CP] = [DCF] = [ACT] = 20 μ M.

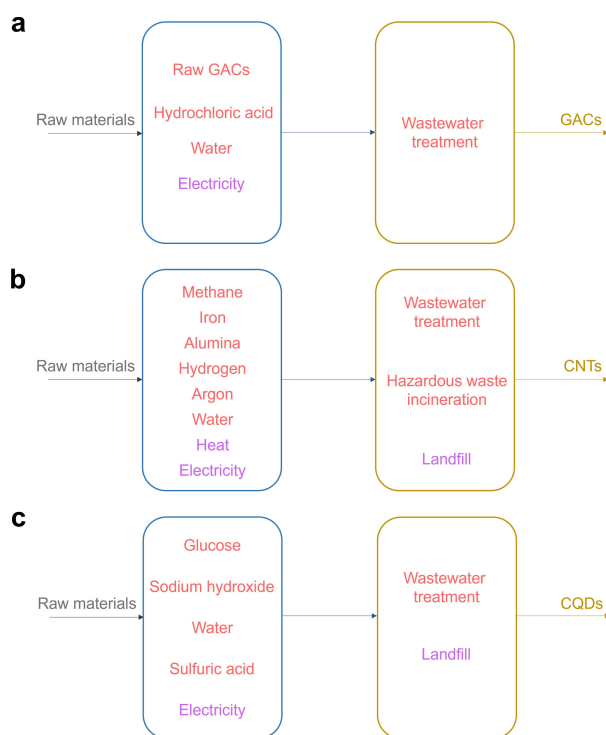


309

310 **Supplementary Fig. 42.** The BPA degradation efficiency of the E-CQDs/PI system in different water

311 matrices. Experimental conditions: $[Cl^-] = [NO_3^-] = [HCO_3^-] = 10 \text{ mM}$, $[HA] = 10 \text{ mg L}^{-1}$.

312



313

314 **Supplementary Fig. 43. a-c,** The material and energy flow during the synthesis processes of granular
 315 activated carbon (GACs) (a), carbon nanotubes (CNTs) (b), and CQDs (c).

316 The LCA of GACs, CNTs, and CQDs was conducted using Simapro software (version 9.0) with
 317 the Ecoinvent 3.5 database. We evaluated the environmental impact of the process of synthesizing
 318 1kg of three different materials. The material and energy flow during the synthesis process is shown
 319 in Figure S7. The blue boxes indicated the input raw materials and energy, while the yellow boxes
 320 showed the waste and disposal processes. The standard for measuring environmental impact was
 321 adopted as ReCiPe 2016 Midpoint (H) V1.08 / World (2010).

322

323 **Supplementary Tables**

324 **Table S1.** The molecular orbital energies of CQDs under different electric field intensities

Electric field intensity ($\times 10^6$ a.u.)	Molecular orbital energies of CQDs		
	HOMO energy	LUMO energy	Band gap
	(eV)	(eV)	(eV)
0	-4.69	-2.93	1.76
0.25	-4.68	-2.98	1.70
0.5	-4.64	-3.24	1.40
0.75	-4.65	-3.86	0.79
1.25	-4.58	-4.06	0.52
1.5	-4.54	-4.02	0.52
1.75	-5.08	-4.53	0.55
2	-5.77	-5.34	0.43

325

326

Table S2. The molecular orbital energies of CQDs under different electric field intensities

Elements	Systems	Functional groups	Percentage
C 1s	CQDs	C-SP ²	64.85
		C-O	15.25
		C=O	19.90
	CQDs-PI	C-SP ²	61.16
		C-O	12.06
		C=O	26.78
O 1s	CQDs	O-H	13.71
		C-O	35.41
		C=O	50.88
	CQDs-PI	O-H	10.96
		C-O	28.69
		C=O	49.19
		I-O	11.16

327

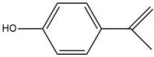
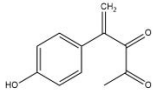
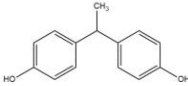
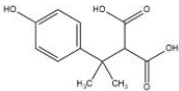
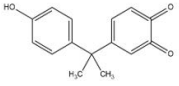
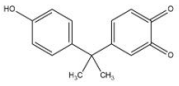
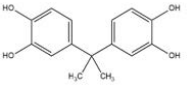
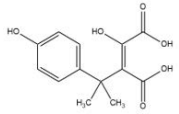
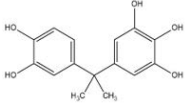
Products	Rt (min)	Calculated m/z	Observed m/z	Formula	Structure
TP-93	10.879	93.0346	93.0338	C ₆ H ₆ O	
TP-107	14.152	107.0139	107.0133	C ₆ H ₄ O ₂	
TP-133	13.149	133.0659	133.0636	C ₉ H ₁₀ O	
TP-189	19.128	189.0557	189.0615	C ₁₁ H ₁₀ O ₃	
TP-227	1.258	227.0714	227.0731	C ₁₄ H ₁₂ O	
TP-237	12.367	237.0768	237.0731	C ₁₂ H ₁₄ O ₅	
TP-241	5.992	241.0870	241.0906	C ₁₅ H ₁₄ O ₃	
TP-243	18.732	243.1027	243.1072	C ₁₅ H ₁₆ O ₃	
TP-259	18.765	259.0976	259.0943	C ₁₅ H ₁₆ O	
TP-265	14.830	265.0718	265.0665	C ₁₃ H ₁₄ O ₆	
TP-275	17.161	275.0925	275.0981	C ₁₅ H ₁₆ O ₅	

Table S4. Fukui index of BPA

Atom	Site	f^-	f^+	f^0
O	1	0.0736	0.0299	0.0517
O	2	0.0736	0.0299	0.0518
C	3	0.0038	-0.0006	0.0016
C	4	0.0479	0.0125	0.0302
C	5	0.0479	0.0125	0.0302
C	6	0.0113	0.0082	0.0098
C	7	0.0113	0.0082	0.0098
C	8	0.0319	0.0493	0.0406
C	9	0.0319	0.0493	0.0406
C	10	0.0306	0.0624	0.0465
C	11	0.0306	0.0624	0.0465
C	12	0.0344	0.0657	0.0501
C	13	0.0344	0.0657	0.0501
C	14	0.053	0.0658	0.0594
C	15	0.053	0.0658	0.0594
C	16	0.054	0.0302	0.0421
C	17	0.054	0.0302	0.0421

332

Table S5. The electrical energy per order (EEO) values of E-CQDs/PI and other systems.

Systems	k_{obs} (min^{-1})	E_{EO} ($\text{kWh m}^{-3} \text{ order}^{-1}$)	References
E-CQDs/PI	0.270	0.068	This work
E-PI	0.050	0.368	This work
E(Ti/SnO ₂ -Sb)	0.240	0.366	Zhou et al. ⁵
E(MMO/Ti)	0.014	5.552	Fuller et al. ⁶
US/FCPs/PMS	0.043	0.473	Ma et al. ⁷
VUV/Fe(III)	0.015	2.17	Yao et al. ⁸
US/PS/H ₂ O ₂ /Fe(II)	0.085	16.2	Kyzas et al. ⁹
UV/O ₃ /TiO ₂	0.080	14.4	Asgari et al. ¹⁰
E(Ti/ β -PbO ₂)	0.064	5.71	Zhang et al. ¹¹

333

Table S6. Specific HPLC analytical parameters for different substrates

Substrates	Mobile phase (A / B)	Proportion	Wavelength (nm)	Flow rate (mL min ⁻¹)
BPF	Water / acetonitrile	50 / 50	276	1.0
Phenol	Water / acetonitrile	50 / 50	270	1.0
BPA	Water / methanol	25 / 75	230	1.0
2,4-DCP	Water / acetonitrile	28 / 72	280	1.0
4-CP	Water / acetonitrile	30 / 70	280	1.0
DCP	Acetic acid (0.1% v/v) / acetonitrile	20 / 80	276	1.0
ACT	Water / acetonitrile	40 / 60	243	1.0
2 - IP	Water / acetonitrile	60 / 40	286	1.0
4 - IP	Acetic acid (0.1% v/v) / methanol	40 / 60	231	1.0

336

- 337 1. Luo, M. F. et al. Electrochemical activation of periodate with graphite electrodes for water
338 decontamination: Excellent applicability and selective oxidation mechanism. *Water Res.* **240**,
339 120128 (2023).
- 340 2. Li, Y. X. Zhang, D. P. Wang, P. F. Qu, J. Y. & Zhan, S. H. Superoxide radicals mediated by high-
341 spin Fe catalysis for organic wastewater treatment. *Proc. Natl. Acad. Sci. U.S.A.* **121**,
342 e2407012121 (2024).
- 343 3. Zhang, T. et al. Overcoming Acidic H₂O₂/Fe(II/III) Redox-Induced Low H₂O₂ Utilization
344 Efficiency by Carbon Quantum Dots Fenton-like Catalysis. *Environ. Sci. Technol.* **56**, 2617–
345 2625 (2022).
- 346 4. Wu, L. L. et al. Self-Driven UV/Periodate Process for Cu-EDTA Decomplexation and In Situ
347 Copper Recovery. *Environ. Sci. Technol.* **60**, 16268–16278 (2026).
- 348 5. Zhou, C. Z. Wang, Y. P. Chen, J. & Niu, J. F. Porous Ti/SnO₂-Sb anode as reactive
349 electrochemical membrane for removing trace antiretroviral drug stavudine from wastewater.
350 *Environ. Int.* **133**, 105157 (2019).
- 351 6. Fuller, M. E. Zhao, Y. W. Hedman, P. C. & Schaefer, C. E. Cathodic electrochemical degradation
352 of legacy (HMX, RDX, TNT) and insensitive (NTO, NQ, DNAN) munitions constituents. *J.*
353 *Hazard. Mater.* **491**, 137789 (2025).
- 354 7. Ma, D. M. et al. Fluorocarbon polymers mediated contact-electro-catalysis activating
355 peroxymonosulfate for emerging pollutants degradation: The key role of fluorine density in
356 electron transfer. *Chem. Eng. J.* **497**, 154996 (2024).

- 357 8. Yao, H. Pei, J. Wang, H. & Fu, J. Effect of Fe(II/III) on tetracycline degradation under UV/VUV
358 irradiation. *Chem. Eng. J.* **308**, 193–201 (2017).
- 359 9. Kyzas, G. Z. Mengelizadeh, N. Saloot, M. K. Mohebi, S. & Balarak, D. Sonochemical
360 degradation of ciprofloxacin by hydrogen peroxide and persulfate activated by ultrasound and
361 ferrous ions. *Colloid Surf. A* **642**, 128627 (2022).
- 362 10. Asgari, E. Sheikhmohammadi, A. Nourmoradi, H. Nazari, S. Aghanaghad, M. Degradation of
363 ciprofloxacin by photocatalytic ozonation process under irradiation with UVA: Comparative
364 study, performance and mechanism. *Process Saf. Environ.* **147**, 356–366 (2021).
- 365 11. Zhang, R. R. et al. Strategy for enhancing the electrocatalytic performance of Ti/ β -PbO₂ anode:
366 Optimizing SnO₂ intermediate layer by Cs doping and application for the efficient removal of
367 mixed fluoroquinolones. *J. Alloy. Compd.* **895**, 162528 (2022).