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

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14 **Abstract**

15 Direct electron transfer (DET) enables selective, matrix-resistant oxidation of organic contaminants,
16 but its efficiency remains constrained by limited electronic tunability of catalysts. Here, we exploit
17 the quantum-confined Stark effect (QCSE) of carbon quantum dots (CQDs) to establish an electric-
18 field-responsive catalytic platform that enables dynamic regulation of electron-transfer processes.
19 Under the external electric field, CQDs undergo QCSE-induced electronic reconstruction, narrowing
20 the bandgap from 1.76 to 0.43 eV and dynamically tuning frontier orbital alignment to facilitate
21 efficient charge transfer. Meanwhile, electric-field-driven migration of charged CQDs creates a
22 spatially optimized reaction microenvironment, directing the catalytic process toward an anodic DET
23 pathway and enhancing pollutant degradation kinetics by up to 7.86-fold. Spectroscopic analyses and
24 theoretical calculations further reveal that QCSE triggers dynamic reconstruction of the CQDs
25 interface, where surface hydroxyl groups undergo deprotonation and oxygen-centered coupling with
26 oxidant to establish efficient electron-transfer channels. The synergistic regulation of electronic states,
27 reactant transport, and interfacial interactions enables DET-coupled non-radical oxidation with $\text{O}_2^{\bullet-}$
28 and $^1\text{O}_2$ generation for accelerated pollutant removal. This work establishes an electric-field-
29 responsive quantum catalytic platform and provides a strategy for designing dynamically
30 programmable electron-transfer interfaces toward sustainable water remediation.

31 **Keywords:** Quantum confined Stark effect; Direct electron transfer; Carbon quantum dots; Frontier
32 orbital alignment.

33 Main

34 Direct electron transfer (DET) has emerged as a pivotal mechanism for the selective removal of
35 emerging organic contaminants (EOCs) from complex aquatic environments. Mechanistically, the
36 oxidant (e.g., hydrogen peroxide (H_2O_2), persulfate (PS), and periodate (PI)) adsorbs onto the catalyst
37 surface to form an oxidant–catalyst reactive complex. When the oxidation potential of this complex
38 exceeds that of the co-adsorbed micropollutants, electrons are transferred directly from the pollutants
39 to the complex at the interface, bypassing the formation of radicals. This intrinsic characteristic
40 endows the DET process with high selectivity toward electron-rich organics and exceptional
41 resistance to the non-specific scavenging effects of background water constituents^{1, 2}. Furthermore,
42 the activated complex formed during the DET process can simultaneously generate reactive oxygen
43 species (ROS), such as $\text{O}_2^{\bullet-}$ and $^1\text{O}_2$, creating a synergistic degradation pathway that combines the
44 selectivity of the DET process with the oxidative power of specific ROS³.

45 The DET process is governed by two fundamental prerequisites: precise energy-level matching
46 and low-resistance interfacial electron transfer channels. Thermodynamically, the driving force of the
47 DET process originates from the electrochemical potential difference, physically manifested as an
48 energy level offset. Specifically, a favorable energy gradient is established to drive spontaneous
49 electron flow when the highest occupied molecular orbital (HOMO) of the electron-donor exceeds
50 the lowest unoccupied molecular orbital (LUMO) of the electron-acceptor. Kinetically, efficient
51 electron tunneling necessitates effective wave function overlap achieved through strong inner-sphere
52 complexation. This intimate contact fosters robust electronic coupling, creating a low-resistance
53 pathway for ultrafast interfacial electron transfer. Such characteristics are typically pursued by
54 conventional strategies like heteroatom doping and defect engineering, which introduce localized
55 states near the Fermi level ([Fig. 1a](#))^{4, 5}. However, these static modifications suffer from inherent

56 limitations. The synthesis-induced heterogeneity and immutable electronic structures yield rigid band
57 configurations that cannot adapt to diverse pollutant redox potentials⁶. This leads to persistent energy
58 mismatches and deep electron traps, severely restricting precise reaction control and overall DET
59 efficiency.

60 To overcome the limitations of static catalyst design, external field-assisted regulation has
61 emerged as a promising strategy for dynamically tuning electronic structures and catalytic behaviors.
62 Various external fields, including plasma, heat, light, magnetic fields, ultrasound, and gravity, have
63 been explored to enhance ROS generation and pollutant degradation in advanced oxidation processes
64 (AOPs)⁷. Among them, external electric field provides unique opportunities for directly manipulating
65 electronic energy levels with high precision, particularly in quantum-confined nanomaterials. This
66 capability originates from the quantum-confined Stark effect (QCSE), which describes the electric-
67 field-induced redistribution of electronic states and energy-level modulation in nanoscale systems^{8,9}.
68 In quantum-confined materials, QCSE enables dynamic bandgap narrowing and frontier orbital
69 realignment by regulating electron-hole wavefunctions¹⁰. Although widely exploited in
70 optoelectronic technologies, including electro-optical modulators¹¹, quantum light sources¹², and
71 compact spectrometers¹³, the potential of QCSE in environmental catalysis remains largely
72 unexplored. Unlike conventional catalyst engineering strategies that generate fixed electronic
73 configurations, QCSE offers a continuously tunable electronic landscape, enabling on-demand
74 optimization of charge-transfer energetics among catalysts, oxidants, and pollutants ([Fig. 1b](#)).
75 Therefore, identifying quantum-confined materials with highly responsive electronic structures is
76 essential for translating this field-induced electronic tunability into catalytic applications. Carbon
77 quantum dots (CQDs) are promising platforms for such regulation owing to their quantum-confined
78 electronic properties, excellent conductivity, abundant surface functional groups, and large specific

surface areas^{14, 15, 16}. However, their DET activity remains restricted by intrinsic electronic structures and interfacial interactions, limiting dynamic control over electron-transfer pathways. Integrating QCSE with CQDs therefore provides a unique opportunity to transform static carbon catalysts into field-programmable electron-transfer interfaces for efficient environmental remediation.

In this study, we exploit the field-responsive electronic nature of CQDs to construct an electric-field-driven catalytic platform for regulating DET processes in pollutant degradation. We demonstrate that the applied electric field induces QCSE-mediated electronic reconstruction of CQDs, reducing their bandgap from 1.76 to 0.43 eV and enabling frontier orbital modulation for optimized charge-transfer energetics. Meanwhile, the electric field regulates the spatial distribution of charged species, directing the reaction toward an anodic DET pathway and enhancing pollutant degradation kinetics by up to 7.86-fold. Furthermore, multiphysics simulations reveal that the electric field drives the anodic co-enrichment of catalytic components and oxidants, creating a favorable microenvironment for the promoted anodic DET process. Spectroscopic analyses and theoretical calculations further uncover a QCSE-induced dynamic reconstruction of the catalytic interface, where surface hydroxyl groups evolve into oxygen-centered electron-transfer channels through interfacial deprotonation and orbital coupling. This synergistic regulation of quantum electronic states, reactant transport, and catalytic interfaces enables DET-coupled non-radical oxidation with rapid kinetics, low energy consumption, and broad environmental applicability, establishing an electric-field-responsive quantum catalytic platform for sustainable water remediation.

Results and discussion

QCSE in CQDs under the external electric field

CQDs were synthesized via a bottom-up self-assembly strategy ([Fig. 2a](#)). During the synthesis, glucose underwent polymerization and structural transformation under ultrasonication, leading to the

102 formation of nanoparticles. The formed CQDs exhibit a low-dimensional architecture and distinct
103 spectral properties. TEM and AFM imaging confirmed that the CQDs maintain a well-dispersed and
104 isolated nanoparticle morphology with 4.35 nm of particle size (Fig. 2b and Supplementary Fig. 1),
105 which is crucial for preserving intrinsic quantum confinement effects¹⁷. This confinement dictates
106 both the optical and electronic behavior of the CQDs. The optical characterization showed a sharp
107 emission peak at 440 nm (excitation peak at 370 nm) and a UV-Vis absorption peak at 275 nm,
108 corresponding to a discrete bandgap and $\pi \rightarrow \pi^*$ transitions, respectively (Supplementary Fig. 2 and
109 Supplementary Fig. 3). Such well-defined energy states are characteristic of quantum-confined
110 systems and result in an electron distribution that is highly susceptible to perturbation¹⁸. Within the
111 nanoscale regime, this quantum confinement dramatically amplifies the sensitivity of internal electron
112 distributions to external electric fields, manifesting as a pronounced phase shift in electrostatic force
113 microscopy (EFM) signals^{19, 20}. As shown in Fig. 2c and Supplementary Fig. 4–8, it reveals a
114 parabolic dependence of the EFM phase shift on the tip bias voltage ($\Delta\phi \propto V_{\text{EFM}}^2$), indicating a
115 second-order electrostatic response associated with field-induced polarization of quantum-confined
116 CQDs. Notably, the vertex of the parabolic curve shifts to -0.294 V, indicating an intrinsic negative
117 surface charge on the CQDs arising from the deprotonation of surface functional groups²¹.
118 Consistently, DFT calculations demonstrate another quadratic increase in the induced dipole moment
119 of CQDs as a function of the external electric field (Fig. 2d), directly demonstrating that the
120 experimentally observed EFM response originates from the second-order polarization of confined
121 electronic states. These results establish the occurrence of a quadratic Stark response in CQDs, where
122 external electric fields drive electron redistribution and polarization²².

123 The electronic polarization effect stems from the spatial reorganization of the electronic state
124 density, especially for the electrons at the frontier orbital energy levels²³. The local density of states

(LDOS) along the dipole axis of the CQDs depicts significant LDOS redistribution under the external field (Fig. 2e and Supplementary Fig. 9). Specifically, the electron density in the HOMO diminishes, while that in the LUMO intensifies along the dipole direction. This asymmetric redistribution causes a spatial separation of the electron and hole wavefunctions along the electric field, leading to substantial Stark shifts that drive the observed energy level modulation. The in situ photoluminescence (PL) responses of CQDs under varying electric potentials demonstrated that the application of an external field triggers a pronounced quenching of the PL intensity accompanied by a distinct redshift in the emission peak from 565 nm to 580 nm (Fig. 2f). This spectral shift serves as direct evidence of the QCSE-induced narrowing of the effective bandgap, which causes the reduction of the excitation threshold^{24, 25}. Theoretical calculations of the singlet excited state reveal a dramatic reduction in excitation energy from 1.306 eV to 0.149 eV, concurrent with a reconfiguration of the active molecular orbitals (Fig. 2g and Supplementary Fig. 10–12). Collectively, the low-dimensional CQDs exhibit intrinsic quantum confinement features. Such quantum characteristics induce a substantial spatial reconfiguration of electron density under external electric fields, leading to pronounced Stark shifts in energy levels, which provide a solid mechanistic basis for their dynamic catalytic behavior.

QCSE-induced non-intrinsic DET process for decontamination

The external electric field is generally applied across both anodic and cathodic interfaces, yet the spatial distribution of QCSE-induced electronic regulation remains elusive. To determine the preferential region where CQDs experience electric-field modulation, spatially resolved open-circuit potential (OCP) measurements were first performed. As shown in Fig. 3a and Supplementary Fig. 13, a pronounced potential gradient was observed in the CQDs-containing electrolyte, with the region adjacent to the anode exhibiting the largest potential shift. This spatially dependent electrochemical

response indicates that the electronic states of CQDs are more strongly regulated near the anodic interface, suggesting a preferential activation of QCSE-mediated electronic modulation in this region. Based on this observation, the contribution of anodic QCSE regulation to pollutant degradation was further evaluated using BPA and PI as the model contaminant and oxidant, respectively. As shown in [Fig. 3b](#) and Supplementary Fig. 14, the introduction of CQDs substantially accelerated BPA degradation in the anodic E-CQDs/PI system across the entire current range from 10 to 50 mA, with the corresponding rate constants enhanced by 2.57-, 3.56-, 6.56-, 6.24-, and 7.86-fold compared with the CQDs-free E/PI system, respectively. These results demonstrate that anodic QCSE regulation of CQDs effectively enhances PI activation, thereby accelerating pollutant degradation. To elucidate the degradation mechanism occurring in the anodic compartment, a series of reactive species quenching experiments were subsequently performed. As shown in [Fig. 3c](#) and Supplementary Fig. 15, radical quenching experiments using TBA (scavenger for $\cdot\text{OH}$, $k = 3.8\text{--}7.6 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$) indicated a negligible role of $\cdot\text{OH}$ in the oxidation process²⁶. Conversely, the degradation efficiency was significantly suppressed upon the introduction of $\text{K}_2\text{Cr}_2\text{O}_7$ (scavenger of electron, $k = 2.9\text{--}6.0 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$), FFA (scavenger of $^1\text{O}_2$, $k = 1.2 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$), and *p*-BQ (scavenger of $\text{O}_2^{\cdot-}$, $k = 0.9\text{--}1.0 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$), identifying non-radical process as the dominant BPA degradation route^{27, 28 29}.

To elucidate the non-radical pathway responsible for BPA degradation at the anode, the occurrence of DET was first investigated by monitoring the OCP under different applied currents. As shown in [Fig. 3d](#), the OCP gradually shifted toward more positive potentials upon the addition of PI, followed by a negative shift after the introduction of BPA. These sequential potential changes provide direct electrochemical evidence for spontaneous electron extraction from BPA and subsequent electron acceptance by PI, indicating the occurrence of a DET process³⁰. To further verify that the observed reaction originates from electric-field-induced electronic-state modulation rather than direct

171 electrolysis, a membrane-separated salt-bridge reactor was constructed (Fig. 3e). In this configuration,
172 BPA/CQDs and PI were spatially separated to prevent direct molecular contact while preserving the
173 electric-field environment. As shown in Fig. 3f, a distinct current decrease was observed only in the
174 presence of both BPA and CQDs, whereas control experiments lacking either BPA or CQDs exhibited
175 nearly unchanged current responses. These results demonstrate that the QCSE-induced electronic-
176 state modulation of CQDs promotes electronic coupling between BPA and PI, enabling efficient field-
177 driven DET³¹. Considering that $O_2^{\bullet-}$ and $^1O_2$ serve as additional oxidative contributors beyond the
178 DET pathway, nitro blue tetrazolium chloride (NBT) probing and electron spin resonance (EPR)
179 measurements were conducted to verify their generation in the E-CQDs/PI system. As shown in Fig.
180 3g and Fig. 3h, a distinct increase of the UV absorption peak at 560 nm, as well as a triple peak (1:1:1)
181 representing TEMPO, was observed during the NBT chemical probe experiment and EPR analysis in
182 the E-CQDs/PI system, respectively ^{32, 33}. Furthermore, the addition of $K_2Cr_2O_7$ markedly suppressed
183 both the NBT and TEMPO signals, demonstrating that the formation of $O_2^{\bullet-}$ and $^1O_2$ originates from
184 the DET process.

185 Collectively, these findings demonstrate that the QCSE markedly enhances the BPA degradation
186 performance of the E-CQDs/PI system by regulating the electric-field-driven anodic reaction (Fig.
187 3i). The anodic process is dominated by a non-radical DET pathway, in which electrons are directly
188 extracted from BPA to initiate its oxidation. Meanwhile, the DET process activates PI to generate $O_2^{\bullet-}$
189 and $^1O_2$ as secondary oxidizing species, further promoting BPA degradation. The synergistic
190 integration of DET and reactive oxygen species generation ultimately accounts for the superior
191 oxidation performance of the E-CQDs/PI system.

192 **The intrinsic mechanism of the QCSE driving the non-intrinsic DET process**

193 To understand the origin of the anodic preference in the electric-field-enhanced degradation process,
194 the spatial transport behavior of charged reactants under the applied electric field was first
195 investigated. The solution conductivity decreased markedly from 106 to 49 $\mu\text{S cm}^{-1}$ after introducing
196 CQDs ([Fig. 4a](#)), indicating the active participation of charged CQDs in electric-field-driven migration.
197 As negatively charged CQDs and PI experience electrophoretic forces under the electric field, they
198 undergo directional migration toward the anodic region, resulting in their spatial redistribution within
199 the electrochemical system. Multiphysics simulations based on the practical single-cell
200 electrochemical configuration further elucidated the mechanism underlying PI redistribution under
201 the external electric field (Supplementary Fig. 16). Owing to its negative charge, PI underwent
202 continuous electromigration from the cathode towards the anode, resulting in a pronounced
203 concentration polarization across the cell (Supplementary Fig. 17–20). Consistent with this migration
204 behavior, [Fig. 4b](#) and Supplementary Fig. 21 revealed a transient PI concentration gradient,
205 characterized by progressive depletion at the cathode and accumulation near the anode within seconds.
206 This asymmetric redistribution selectively enriches PI at the CQD-containing anodic interface while
207 limiting PI availability at the cathode, thereby suppressing competing cathodic PI activation.
208 Consequently, the electric-field-induced spatial regulation of PI and CQDs establishes a favorable
209 microenvironment for interfacial electron coupling and DET processes ([Fig. 4c](#) and Supplementary
210 Fig. 22).

211 After establishing the electric-field-driven spatial redistribution of charged reactants, the
212 regulation of CQDs' electronic properties by the QCSE was further investigated to clarify its
213 contribution to the DET process. The introduction of CQDs significantly increased the electrode
214 capacitance from 354 to 399 $\mu\text{F cm}^{-2}$ ([Fig. 4d](#) and Supplementary Fig. 23), indicating enhanced
215 interfacial charge-storage capability and electron accommodation under electrochemical conditions.

216 This increased charge-storage capacity provides a favorable electronic environment for subsequent
217 electron transfer. Consistently, the incorporation of CQDs resulted in a pronounced increase of 0.146
218 mA cm⁻² in the peak current density ([Fig. 4e](#)), demonstrating accelerated heterogeneous electron
219 transfer between CQDs and PI. These field-dependent electrochemical responses originate from
220 QCSE-induced electronic reconstruction, which dynamically modulates the charge-transfer
221 properties of CQDs and establishes an electronically favorable interface for efficient electron
222 exchange.

223 To further elucidate the molecular origin of the QCSE-triggered DET process, the evolution of
224 CQDs' frontier orbitals under different electric-field intensities was investigated. Thermodynamically,
225 such efficient electron transfer necessitates a favorable energy alignment wherein the donor's
226 occupied states lie energetically higher than the acceptor's unoccupied states¹⁶. By tracking the
227 response of CQDs' frontier orbitals driven by the electric field, the mechanism behind the QCSE-
228 triggered DET was elucidated. [Fig. 4f](#) demonstrates that both HOMO and LUMO energies of CQDs
229 exhibit strong field dependence. As the electric field intensity increases, the bandgap systematically
230 narrows from 1.76 eV to 0.43 eV, significantly lowering the barrier for intra-particle electron transport
231 (Supplementary Table S1). Crucially, under high potential conditions, the molecular orbitals of CQDs
232 shift to achieve energetic matching among BPA, CQDs, and PI. This precise alignment establishes a
233 cascaded energy pathway through which electrons migrate from the HOMO of BPA to the LUMO of
234 CQDs, and subsequently transfer to the LUMO of PI. Such electric field-induced energy alignment
235 facilitates non-intrinsic DET processes, providing a solid foundation for the highly efficient
236 degradation of BPA within the E-CQDs/PI system.

237 While QCSE establishes the thermodynamic driving force for electron transfer, the abundant
238 surface functional groups serve as critical anchoring sites that establish the electron transfer channels

required for the DET process³⁴. 2D-COS analysis of FTIR spectra revealed three positive auto-peaks at 950–1200 cm⁻¹ ($\nu_{\text{C-O}}$), 1600–1700 cm⁻¹ ($\nu_{\text{C=O}}$), and 2950–3600 cm⁻¹ ($\nu_{\text{O-H}}$), demonstrating that both surface carboxyl (–COOH) and –OH groups participate in PI adsorption (Supplementary Fig. 24). However, the asynchronous spectrum exhibited a negative cross-peak at (1600–1700 / 2950–3600) coinciding with the positive synchronous peak, which demonstrated the preferential interaction between PI and –OH groups rather than –COOH groups according to Noda's rules (Fig. 4g)³⁵. This selective binding is attributed to the higher positive electrostatic potential of H atoms in –OH, as evidenced by Electrostatic potential (ESP) calculations (Supplementary Fig. 25). Furthermore, reduced density gradient (RDG) analysis corroborated the stronger attractive interactions in the –OH configuration (Fig. 4h, Supplementary Fig. 26, and Supplementary Fig. 27).

Following the initial surface enrichment, the catalytic interface undergoes a dynamic reconstruction that evolves from physical adsorption to robust chemical bonding. XPS survey spectra confirmed PI adsorption by revealing a distinct iodine signal on the CQD surface (Supplementary Fig. 28). Concurrently, a marked decrease in O–H peak intensity indicated surface deprotonation (Supplementary Table S2 and Supplementary Fig. 29), a finding further supported by the pH drop observed upon mixing PI with CQDs (Supplementary Fig. 30). Complementing this, acid-base titration confirmed a significant rise in anionic functional group concentration at pH > 5 (Supplementary Fig. 31)³⁶. This accumulation of surface negative charge manifested as a notable reduction in zeta potential (Supplementary Fig. 32). The interfacial charge reconstruction induced by the QCSE was further elucidated through overlap population density of states (OPDOS) analyses. As shown in Supplementary Fig. 33, the O 2p orbitals of deprotonated –O⁻ and the I 5d orbitals of PI are located within a similar energy range, resulting in pronounced orbital overlap that favors interfacial electron delocalization and bond formation³⁷. In contrast, only negligible orbital overlap was

262 observed between deprotonated COO^- and PI, indicating a much weaker electronic interaction.
263 Consistent with the OPDOS analysis, the electron localization function (ELF) maps ([Fig. 4i](#)) revealed
264 pronounced electron localization at the O^-/PI interface, indicative of covalent bond formation,
265 whereas only weak electron localization was observed for the COO^-/PI configuration ³⁸. These
266 results demonstrate that the superior orbital compatibility of the O^- active sites facilitates interfacial
267 charge redistribution, thereby providing a favorable electronic configuration for the subsequent direct
268 electron transfer process. These findings establish surface OH as a dynamic two-stage adsorption
269 site: long-range hydrogen bonding initiates PI enrichment from the bulk solution, and subsequent
270 deprotonation creates an oxygen-centered covalent bridge that serves as the low-resistance electron
271 transfer channel (Supplementary Fig. 34).

272 In summary, these results reveal that the electric field regulates the non-intrinsic DET process
273 through a synergistic spatial–electronic modulation strategy. At the macroscopic level, the electric
274 field drives the directional migration and redistribution of charged CQDs and PI, creating a PI/CQD-
275 enriched anodic microenvironment while suppressing the cathodic DEA pathway due to reactant
276 depletion. At the microscopic level, the QCSE dynamically reconstructs the electronic structure of
277 CQDs by tuning frontier orbital energies, narrowing the bandgap and optimizing the energetic
278 alignment among BPA, CQDs, and PI, thereby lowering the barrier for electron transfer. Furthermore,
279 the surface hydroxyl groups of CQDs undergo adaptive interfacial reconstruction, evolving from
280 hydrogen-bond-mediated PI enrichment to deprotonated oxygen-centered covalent bridges that
281 provide efficient electron-transfer channels. This coupling of electric-field-driven spatial regulation,
282 QCSE-induced electronic engineering, and interfacial orbital optimization enables highly efficient
283 non-intrinsic DET, ultimately accounting for the superior BPA degradation performance of the E-
284 CQDs/PI system.

285 **Practical applicability of the QCSE-induced E-CQDs/PI system**

286 To evaluate the practical applicability of the QCSE-enabled catalytic platform, BPA degradation was
287 assessed in an integrated single-cell electrochemical configuration. As shown in Supplementary Fig.
288 35, the E-CQDs/PI system achieved a k_{obs} of 0.270 min^{-1} , representing 270-, 67.5-, and 5.29-fold
289 enhancements over E-CQDs, CQDs/PI, and E/PI systems, respectively. These results demonstrate the
290 synergistic effect of electric-field regulation and CQDs-mediated PI activation under realistic
291 conditions. The transformation pathways and toxicity evolution of BPA were subsequently
292 investigated to assess the environmental consequence of this enhanced degradation. According to the
293 UHPLC-QTOF-MS/MS analysis in ESI positive mode, eleven degradation products were identified
294 during BPA oxidation (Supplementary Table S3 and Supplementary Fig. 36). Furthermore, Fukui
295 index analysis was employed to determine the preferential reactive sites and functional groups of BPA
296 (Supplementary Table S4 and Supplementary Fig. 37)³⁹. The calculated Fukui index revealed that O1,
297 O2, C4, C5, C14, C15, C16, and C17 within the phenolic moieties exhibited relatively higher f^+ values,
298 indicating their susceptibility toward electrophilic attack. Accordingly, BPA degradation proceeded
299 through sequential hydroxylation, demethylation, C–C bond cleavage, and oxidative ring-opening
300 reactions ([Fig. 5a](#)), resulting in progressive destruction of the aromatic structure and generation of
301 smaller oxygenated intermediates. Such stepwise molecular transformation substantially decreased
302 the environmental risks associated with BPA-derived products. Consistently, Ecological structure
303 activity relationships (ECOSAR) analysis demonstrated that the predicted acute toxicity toward fish,
304 daphnia, and green algae continuously declined during BPA oxidation, confirming effective
305 detoxification throughout the degradation process ([Fig. 5b](#))⁴⁰. Moreover, negligible formation of
306 iodine-containing by-products, including HOI and I_2 , was detected in the E/PI and E-CQDs/PI
307 systems (Supplementary Fig. 38), further verifying the environmentally compatible nature of PI

308 activation⁴¹. These findings demonstrate that the E-CQDs/PI system enables not only efficient
309 pollutant removal but also controlled conversion toward less hazardous products.

310 Following the confirmation of efficient degradation and detoxification, the practical applicability
311 of the E-CQDs/PI system was further assessed by comparing its catalytic activity and energy
312 efficiency with representative advanced oxidation processes reported in the literature⁴². As shown in
313 [Fig. 5c](#) and Supplementary Table S5, the proposed system simultaneously achieved one of the highest
314 k_{obs} and the lowest electrical energy consumption ($E_{\text{E/O}} = 0.068 \text{ kWh m}^{-3} \text{ order}^{-1}$) among reported
315 photocatalytic, Fenton-like, and electrochemical oxidation technologies. This favorable combination
316 of rapid kinetics and low energy demand highlights the advantage of the QCSE-driven catalytic
317 strategy over conventional oxidation processes. Notably, the enhancement induced by CQDs was
318 independent of electrode configuration. When the Ni foam electrode was replaced with Zn foam, Cu
319 foam, Ti foam, graphite plate, or carbon felt, the E-CQDs-containing systems consistently exhibited
320 higher BPA degradation efficiency than CQD-free controls ([Fig. 5d](#) and Supplementary Fig. 39),
321 demonstrating that QCSE-mediated PI activation does not rely on specific electrode materials.

322 The general applicability of this strategy was further validated using structurally diverse organic
323 pollutants. Specifically, the E-CQDs/PI system maintained efficient removal of phenol (PN),
324 bisphenol F (BPF), 2,4-dichlorophenol (2,4-DCP), 4-chlorophenol (4-CP), diclofenac (DCF), and
325 acetaminophen (ACT) ([Fig. 5e](#) and Supplementary Fig. 40), demonstrating the broad applicability of
326 QCSE-enabled PI activation toward diverse contaminants. In addition, the system retained high BPA
327 removal efficiency over a wide pH range from 3.0 to 9.0 (Supplementary Fig. 41) and exhibited strong
328 resistance against representative water matrix components, including Cl^- , NO_3^- , HCO_3^- , and humic
329 acid ([Fig. 5f](#) and Supplementary Fig. 42), indicating its robustness under complex environmental
330 conditions.

331 Finally, the environmental sustainability of the proposed technology was assessed through life
332 cycle assessment (LCA) based on 18 environmental descriptors, comparing the synthesis impacts of
333 CQDs with two representative carbon materials (details provided in Supplementary Fig. 43)⁴³. As
334 shown in [Fig. 5g](#), CQDs exhibited consistently lower environmental impacts than granular activated
335 carbon (GAC) and carbon nanotubes (CNTs), which can be attributed to their mild and
336 environmentally benign preparation route. Collectively, the combination of high catalytic efficiency,
337 low energy consumption, broad applicability, operational robustness, and effective detoxification
338 demonstrates that the E-CQDs/PI system represents a sustainable and practically viable strategy for
339 electrochemical water purification.

340 **Discussion**

341 In this study, we have successfully established an electric-field-responsive quantum engineering
342 strategy that harnesses the QCSE of CQDs to enable a non-intrinsic DET pathway in the E-CQDs/PI
343 system. The existence of QCSE-induced electronic polarization was verified through EFM, in situ PL
344 measurements, and DFT calculations, revealing electric-field-dependent charge redistribution and
345 frontier orbital modulation within CQDs. This QCSE-induced electronic reconstruction enables
346 CQDs to function as field-responsive electron mediators for efficient DET. Conductivity analysis and
347 multiphysics simulations further demonstrate that the applied electric field drives the directional
348 migration of charged CQDs and PI, generating an anodic microenvironment favorable for the DET
349 process. Current-dependent OCP measurements and frontier orbital calculations reveal that QCSE
350 dynamically regulates the HOMO/LUMO energy levels of CQDs, optimizing the energetic alignment
351 among BPA, CQDs, and PI to reduce charge-transfer barriers. Moreover, FTIR 2D-COS spectra,
352 surface charge analysis, and OPDOS/ELF calculations demonstrate that QCSE induces adaptive
353 interfacial reconstruction through hydroxyl deprotonation and oxygen-centered electronic coupling

354 with PI, creating low-resistance electron-transfer channels. The synergistic integration of QCSE-
355 driven electronic regulation, electric-field-mediated spatial redistribution, and interfacial orbital
356 optimization enables DET-coupled non-radical oxidation for efficient pollutant removal. The E-
357 CQDs/PI system further exhibits low energy consumption, excellent stability, broad pH adaptability,
358 and applicability toward diverse electrode materials and contaminants. This work provides a general
359 strategy for transforming quantum carbon materials into field-programmable catalytic interfaces for
360 sustainable electrochemical remediation.

361 **Methods**

362 **Chemicals and Materials**

363 All chemicals were used as received without further purification. The details of chemical reagents
364 were listed in the supplementary information.

365 **Preparation of CQDs**

366 CQDs were prepared via the one-step alkaline coupling ultrasonic method. Specifically, 45 g of
367 anhydrous α -glucose was dissolved in 100 mL of deionized water and then sonicated for 3 h. After
368 that, the crude sample was adjusted to pH = 7 with H₂SO₄. The obtained dark brown liquid was treated
369 with a dialysis bag (MWCO 1000) for 12 h, and the dialyzed solution was made up to 250 mL as the
370 pristine CQDs solution.

371 **Experiments**

372 For mechanistic investigations of the QCSE-induced DET process, an H-type electrochemical cell
373 (150 mL) equipped with a proton exchange membrane was employed to spatially separate the anodic
374 and cathodic compartments. A dimensionally stable anode (DSA, 3 cm × 3 cm) and a nickel foam
375 (NF, 3 cm × 3 cm) cathode were fixed in each compartment using electrode clips and positioned
376 parallel to each other. For practical application assessments, a single-compartment glass reactor (150

377 mL) containing both electrodes was used to evaluate the overall pollutant removal performance under
378 integrated electrochemical conditions. Unless otherwise stated, the experiments were carried out
379 under 50 mM Na₂SO₄, 1.5 mM PI, 1.2 g/L CQDs, 20 μM BPA, and pH = 6.5 conditions. The current
380 was maintained at 30 mA with a DC power supply. To evaluate the degradation performance, 1.0 mL
381 of aqueous samples was extracted and filtered through a 0.22 μm filter membrane, and quenched with
382 20 μL Na₂S₂O₃ for HPLC analysis. All experiments were carried out at least twice, and the data were
383 averaged.

384 **Characterization and Analytical Method**

385 The concentration of residual pollutants was measured with HPLC (Agilent 1260, USA) equipped
386 with a UV detector and a C18 separation column (Supplementary Table S6). Transmission electron
387 microscope (TEM, Thermo Fisher Scientific, USA) was employed to observe the morphology of
388 CQDs and obtain their crystal information. Fourier Transform infrared spectroscopy (FTIR, Thermo
389 Fisher Scientific, USA) was conducted to analyze the bonding situation of CQDs. X-ray
390 photoelectron spectroscopy (XPS, Thermo Scientific, USA) was conducted to obtain the oxidation
391 state of the elements within the samples. Electromagnetic resonance spectroscopy (EPR, Bruker, GER)
392 was employed to study the generation of reactive species. BPA degradation products were analyzed
393 with the ultrahigh performance liquid chromatography quadrupole time-of-flight mass spectrometer
394 (UHPLC-QTOF-MS/MS, Thermo Scientific, USA). Atomic force microscope (AFM, Bruker, GER)
395 and electrostatic force microscope (EFM) were employed to characterize the size of CQDs and their
396 charge response in the external electric field, respectively. Ex situ and in situ PL spectra were
397 performed with the spectro-electrochemical integrated test system (SEC, Ivium tec B.V., NL). Cyclic
398 voltammetry (CV) and open-circuit potential (OCP) were tested by the electrochemical working
399 station (Shanghai CH instrument, CN). The solution conductivity was obtained via the electric

400 conductometer (Chengdu Century Ark Science & Technology Co.Ltd., CN). The details of QTOF and
401 electrochemical tests were all presented in the supplementary information.

402 **Theoretical Calculation and Multiphysics Simulations**

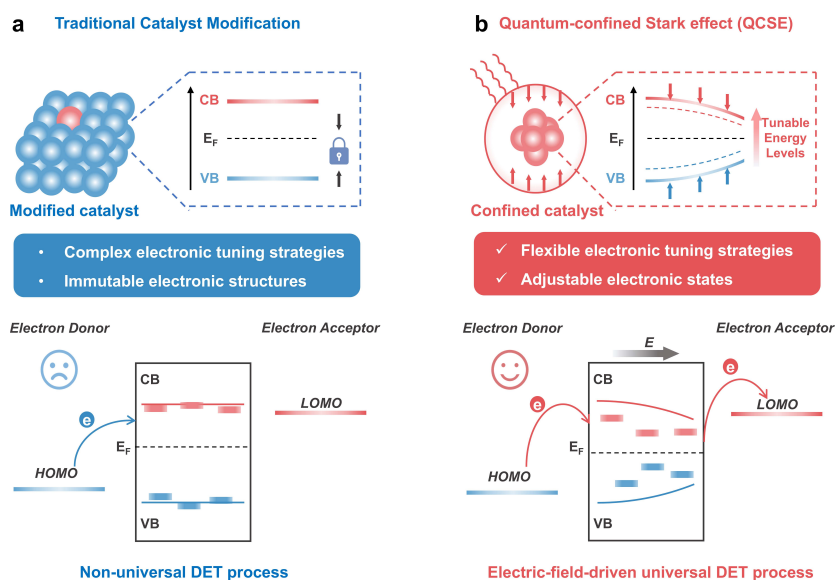
403 The density functional theory (DFT) methods were used to investigate the intrinsic mechanisms of
404 the complexation process, the QCSE under different electric fields, and the molecular orbitals of BPA.

405 The electric field and PI concentration distribution in the electrochemical cell were simulated using
406 the COMSOL software. The details of DFT and COMSOL calculations were presented in the
407 supplementary information.

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Fig. 1 | Conceptual illustration of electronic regulation strategies for DET processes. **a** Traditional catalyst engineering provides static electronic structures, resulting in limited energy-level adaptability between electron donors and acceptors and restricting DET efficiency across different systems. **b** QCSE offers an external-field-driven strategy to dynamically regulate frontier energy levels, enabling adaptive energy alignment and enhanced DET versatility.

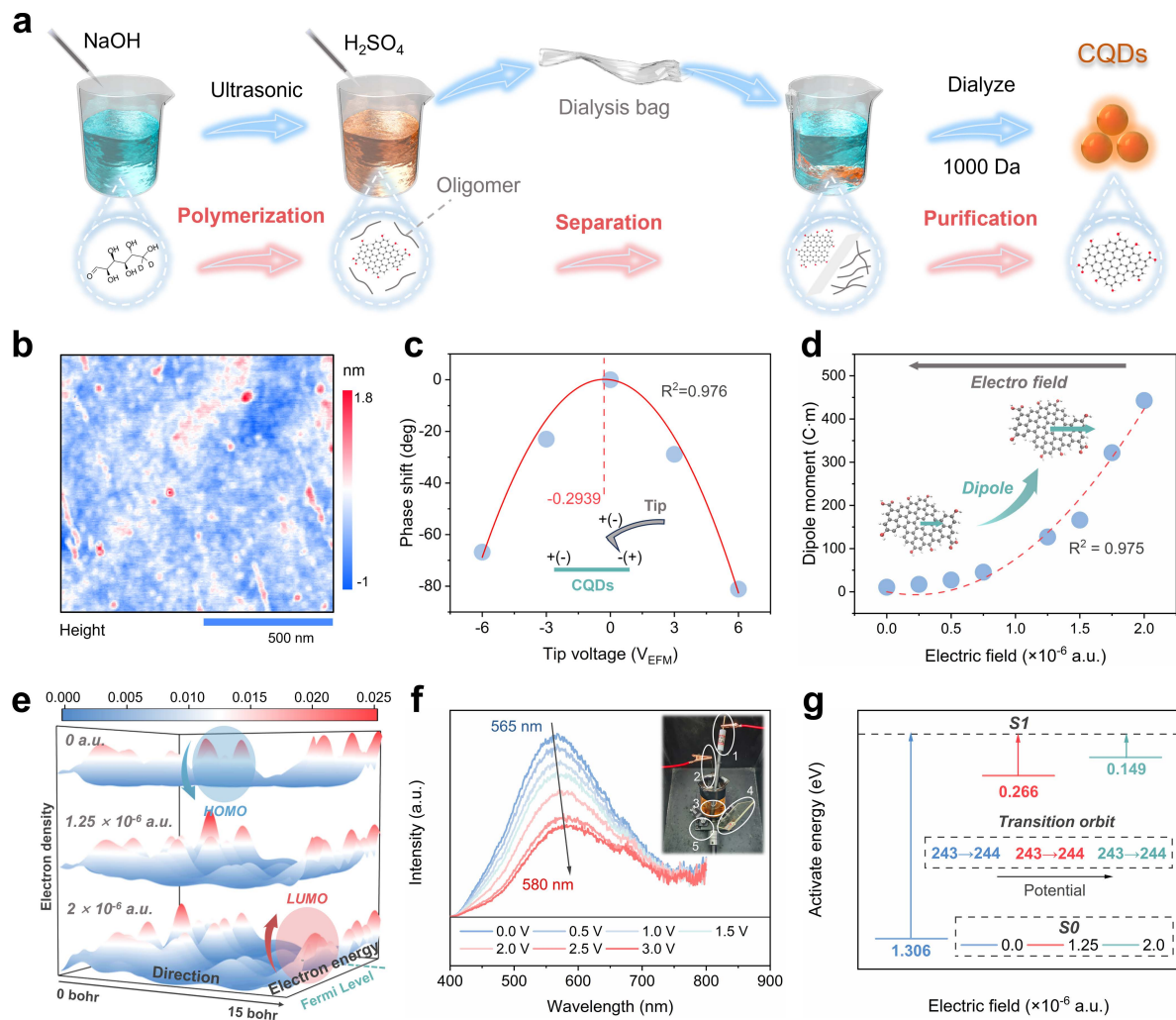


Fig. 2 | QCSE in CQDs. a Schematic illustration of the one-step alkaline coupling ultrasonic synthesis of CQDs. **b** AFM image of CQDs deposited on a mica substrate. **c** Dependence of the phase shift ($\Delta\phi$) on the applied bias voltage (V_{EFM}). The solid line represents the best fit using a polynomial function ($\Delta\phi = aV_{\text{EFM}} + bV_{\text{EFM}}^2$; $a = -1.150^\circ \text{ V}^{-1}$, $b = -2.102^\circ \text{ V}^{-2}$). **d** Variation of the dipole moment (μ) of CQDs as a function of electric field intensity (E). The dashed line represents the best fit using a polynomial function ($\mu = aE + bE^2$; $a = -6.066 \times 10^7 \text{ C m a.u.}^{-1}$, $b = 1.362 \times 10^7 \text{ C m a.u.}^{-1}$). **e** Local density of states (LDOS) of CQDs along the dipole direction under different electric field intensities. **f** In situ PL spectra of CQDs under different applied potentials (Inset image shows the device of the in-situ PL, which was conducted by 1. Graphite electrode; 2. Platinum wire electrode; 3. CQDs solution; 4. Filter; 5. Base). **g** Excitation energies and corresponding excited-state orbitals of CQDs under different electric field intensities.

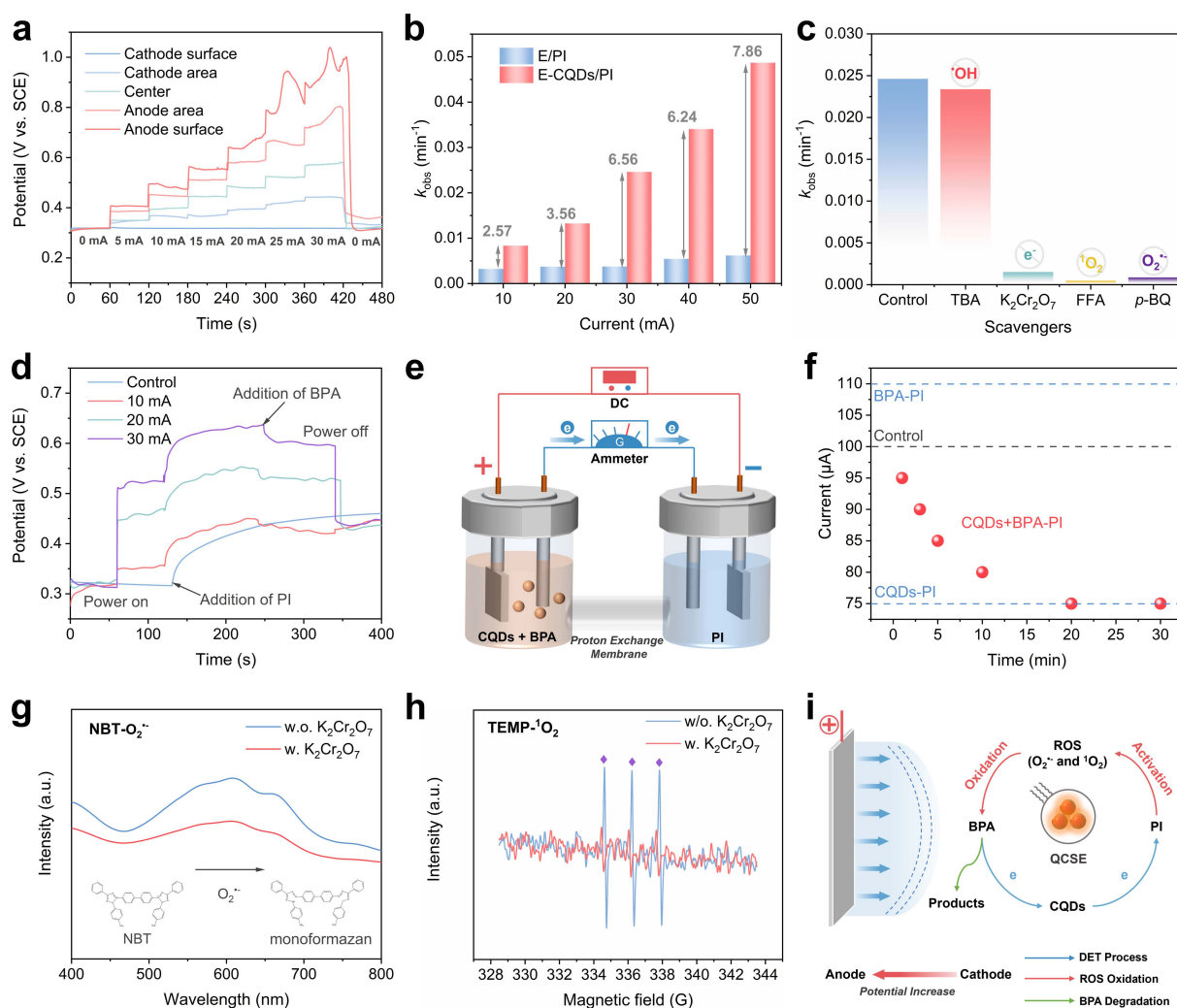


Fig. 3 | QCSE-induced pollutant removal process. **a** Open-circuit potential (OCP) curves of CQDs at different spatial positions under various current intensities. **b** BPA removal performance at the anode in the E-CQDs/PI system under different current intensities. **c** Kinetic analysis of BPA removal in the presence of various scavengers. **d** OCP responses of CQDs after sequential addition of PI and BPA under different current intensities. **e** Schematic illustration of the salt-bridge device. **f** Current response changes in the salt-bridge system. **g** UV-vis spectra of the E-CQDs/PI system using NBT as a probe with and without $K_2Cr_2O_7$ addition. **h** EPR spectra of the E-CQDs/PI system with and without $K_2Cr_2O_7$ addition. **i** Proposed mechanism for QCSE-induced BPA removal.

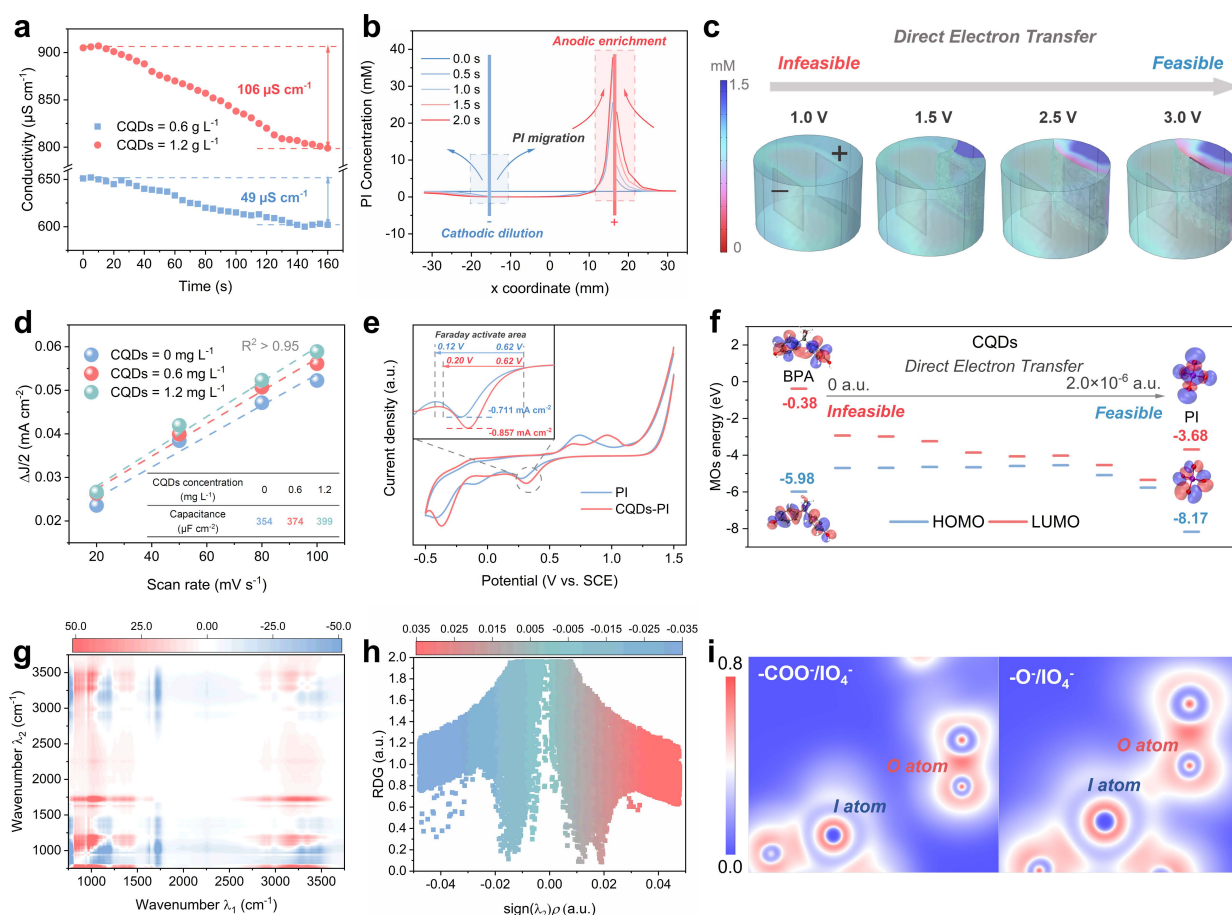
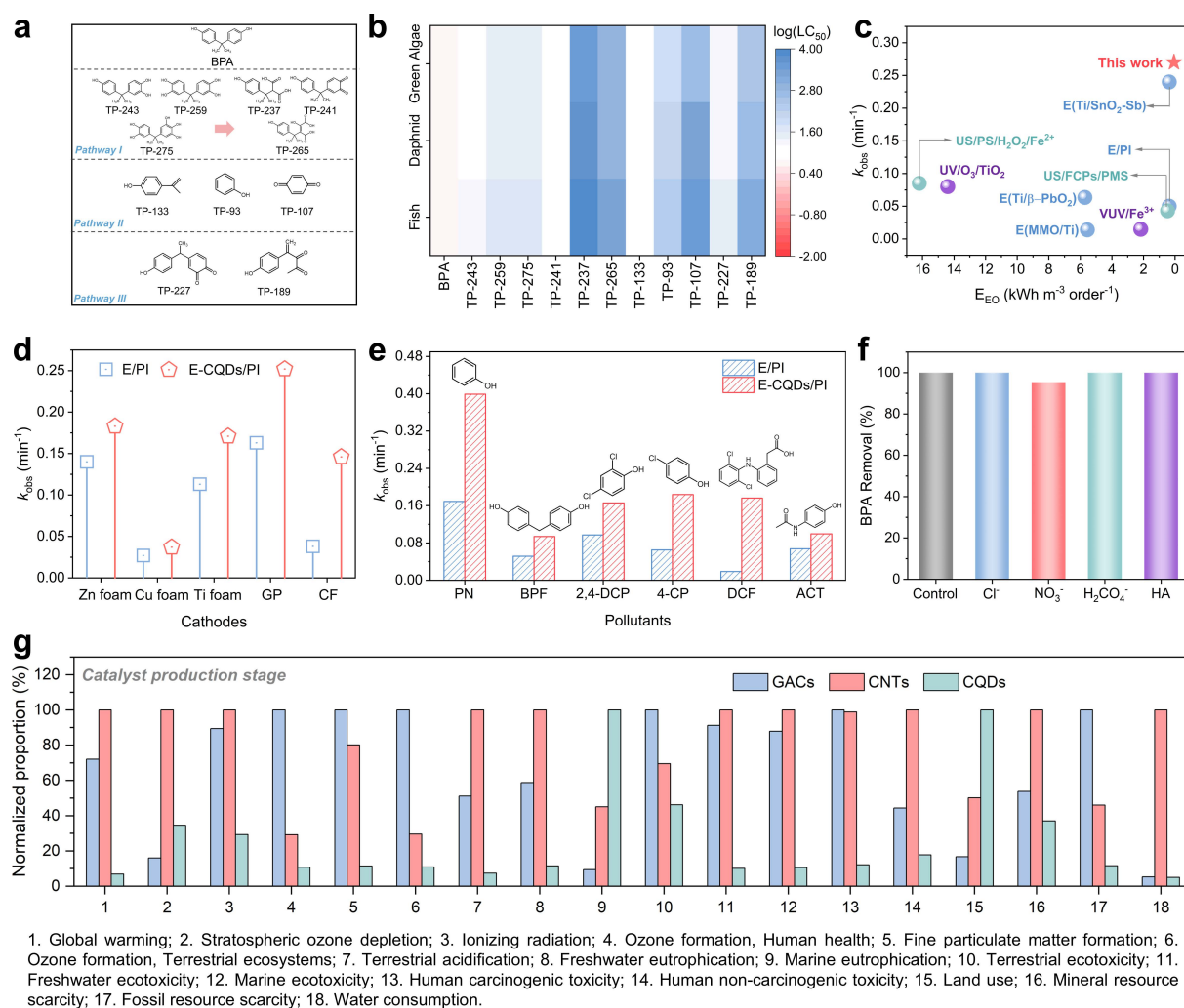


Fig. 4 | Mechanistic insights into QCSE-driven non-intrinsic DET processes. **a** Solution conductivity of CQDs dispersions with different CQDs concentrations. **b** Simulated PI concentration profile along the x-axis at an applied voltage of 2.5 V. **c** PI concentration distributions under different applied potentials and the corresponding PI activation regions (cyan areas indicate the activated regions of PI). **d** Electrode capacitances with different CQDs concentrations. **e** CV curves of the Faradaic region for the PI and CQDs-PI systems (inset: enlarged view of the Faradaic region). **f** Molecular orbital energy-level alignment among BPA, CQDs, and PI under different electric field intensities. **g** Asynchronous two-dimensional correlation spectroscopy (2D-COS) maps derived from FTIR spectra of CQDs-PI complexes. **h** Corresponding reduced density gradient (RDG) versus electron density (ρ) multiplied by the sign of the second largest Hessian eigenvalue (λ_2) for -OH adsorption. **i** Electron localization function (ELF) distributions of PI and CQDs with -O⁻ and -COO⁻ adsorption configurations (higher values indicate stronger electron localization).



1. Global warming; 2. Stratospheric ozone depletion; 3. Ionizing radiation; 4. Ozone formation, Human health; 5. Fine particulate matter formation; 6. Ozone formation, Terrestrial ecosystems; 7. Terrestrial acidification; 8. Freshwater eutrophication; 9. Marine eutrophication; 10. Terrestrial ecotoxicity; 11. Freshwater ecotoxicity; 12. Marine ecotoxicity; 13. Human carcinogenic toxicity; 14. Human non-carcinogenic toxicity; 15. Land use; 16. Mineral resource scarcity; 17. Fossil resource scarcity; 18. Water consumption.

Fig. 5 | Assessment of the practical applicability of the E-CQDs/PI system. a Proposed degradation pathways of BPA in the E-CQDs/PI system. **b** Toxicity assessment of BPA degradation intermediates generated in the E-CQDs/PI system. **c** Comparison of the E-CQDs/PI system with previously reported methods based on k_{obs} and E_{EO} values. **d** BPA removal kinetics in E/PI and E-CQDs/PI systems equipped with different cathode materials. **e** Removal kinetics of various pollutants in the E/PI and E-CQDs/PI systems. **f** BPA removal kinetics of the E-CQDs/PI system in different water matrices. **g** Relative environmental impact of environmentally relevant descriptors for synthesizing 1 kg of GACs, CNTs, and CQDs.

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