

Conjugated donor-acceptor polymer piezocatalysis for hydrogen peroxide generation

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ABSTRACT: Piezocatalysis provides a promising, sustainable route for onsite H_2O_2 production from ubiquitous mechanical energy. However, current piezocatalytic systems are predominantly based on inorganic materials, while organic piezocatalysts have received limited attention. Herein, we report a conjugated donor-acceptor (D-A) polymer prepared via a facile one-step polycondensation method, and systematically explore its piezocatalytic performance for H_2O_2 production. The as-prepared D-A polymer achieves a remarkable piezocatalytic H_2O_2 production rate of 4.3 mmol g^{-1} within 30 min, outperforming the majority of previously reported organic and inorganic piezocatalysts. Experiments and DFT computations demonstrate that the delocalized conjugated backbone facilitates efficient charge migration within the D-A polymer. The spatially segregated frontier molecular orbitals effectively inhibit undesirable charge carrier recombination. Meanwhile, periodic mechanical strain dynamically modulates the reaction thermodynamics through optimizing the adsorption energy of reactants and desorption energy of H_2O_2 . This work not only develops an efficient metal-free organic piezocatalyst for sustainable onsite H_2O_2 synthesis, but also offers critical theoretical guidance for the rational design of advanced organic piezocatalytic materials.

KEYWORDS: Piezocatalysis, Hydrogen peroxide production, Donor-acceptor polymer, Oxygen reduction reaction, Charge separation

1. Introduction

Hydrogen peroxide (H_2O_2) is widely regarded as a multifunctional eco-friendly oxidant and promising liquid fuel, featuring a high mass energy density, with water and oxygen being its sole degradation products^[1,2]. It has been extensively employed across various sectors such as fine chemical manufacturing, environmental restoration, pulp bleaching, and portable fuel cell systems^[3]. Currently, the industrial-scale production of

H_2O_2 is dominated by the classic anthraquinone synthetic route which is plagued by excessive power expenditure, toxic organic waste generation, and complex multi-step operations^[4]. Moreover, the high reactivity and instability of H_2O_2 bring significant safety risks and economic costs to its long-distance transportation and storage^[5]. Therefore, developing a facile, sustainable strategy for onsite H_2O_2 production driven by renewable energy has attracted increasing research attention^[6].

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In recent years, piezocatalysis has evolved into a promising substitute route for sustainable H_2O_2 synthesis [7]. This strategy combines the inherent piezoelectric property of solids with interfacial redox electrochemistry, enabling the direct conversion of ubiquitous ambient mechanical vibration energy (such as water flow, ultrasonic vibration, and acoustic waves) into chemical energy [8]. Piezocatalytic systems are not restricted by specific environmental conditions, and can realize continuous operation in diverse scenarios with no requirement for additional high energy input, showing great application potential in decentralized onsite H_2O_2 production [2]. Nevertheless, the development of piezocatalytic H_2O_2 production is still hindered by the lack of high-performance catalysts. Traditional inorganic piezoelectric materials generally exhibit a weak intrinsic piezoelectric response under mild mechanical excitation, and their rigid structure and poor structural tunability further limit the optimization of their catalytic performance [9]. Organic piezoelectric materials, by contrast, show unique advantages in the field of piezocatalysis, including excellent mechanical flexibility, high structural designability, and tunable intrinsic dipole moment that enables favorable piezoelectric activity under mild conditions [5].

Conjugated donor-acceptor (D-A) polymers, as a class of metal-free organic semiconductor materials, have attracted tremendous interest in the fields of energy storage, photocatalysis, and organic optoelectronics in recent years, owing to their unique merits like customizable skeleton architecture and modifiable electronic band configuration, excellent solution processability, and good mechanical flexibility [10, 11]. The alternating arrangement of electron-donating (D) and electron-accepting (A) units in the polymer backbone can induce a strong intramolecular charge transfer (ICT) effect and permanent dipole moment, which simultaneously facilitate the separation and migration of charge carriers as well as endow the material with an intrinsic piezoelectric response under mechanical deformation [12]. However, research on D-A conjugated polymers for piezocatalytic H_2O_2 production is still in its infancy, and the correlation between their piezoelectric response, charge separation behavior and catalytic performance has not been systematically elucidated [13].

Herein, we report a conjugated donor-acceptor (D-A) polymer prepared via a facile one-step polycondensation route, and systematically explore its piezocatalytic performance for H_2O_2 production. The prepared D-A polymer achieves outstanding H_2O_2 production activity, outperforming most previously reported polymer-based and inorganic piezocatalysts [5], with excellent long-term

cycling stability. Comprehensive mechanistic studies combining control experiments, spectroscopic characterizations alongside first-principles DFT simulations demonstrate that the D-A skeleton enables spatial separation of piezoelectrically generated free charge carriers, that periodic mechanical strain from ultrasonic vibration optimizes reactant activation and product desorption [8], and that the reaction proceeds via a selective two-electron oxygen reduction reaction (ORR) pathway. This work develops an efficient metal-free organic piezocatalyst for sustainable H_2O_2 synthesis, and provides a facile route to boost the catalytic efficiency of organic piezocatalytic materials [14].

2. Experimental sections

2.1. Materials

All reagents were of analytical grade and were used as received without further purification.

2.2. Preparation of D-A polymers

Donor-acceptor (D-A) polymers were fabricated via thermal polycondensation between carboxyl and amino groups. Specifically, 8 mmol of melamine (MA) and 8 mmol of terephthalic acid (TPA) were charged into a single-necked flask containing 60 mL of dimethyl sulfoxide (DMSO). Subsequently, the reaction vessel was placed into an oil bath and maintained at 60 °C for 30 min with continuous stirring to ensure complete dissolution of the raw monomers. Subsequently, the reaction temperature was gradually elevated to 150 °C, and the polycondensation proceeded at this temperature for 72 h. Upon completion of the polymerization, the crude product was rinsed in turn using methanol and hot deionized water for multiple cycles to remove unreacted monomers and residual solvent. The purified product was subsequently vacuum-dried at 60 °C for 24 h to obtain the target polymer, denoted as MTP-150. For comparison, a control sample (designated as MTP-120) was prepared following an identical procedure, with the only difference that the reaction temperature was adjusted to 120 °C.

2.3. Characterization and computational details

Complete characterization and computational details are provided in Text S1 and Text S2 (Supporting Information).

2.4. Piezocatalytic H₂O₂ production

Unless explicitly specified otherwise, all piezocatalytic measurements were carried out under the same experimental conditions. In a typical test, a 60 mL open glass reaction tube was used as the reactor, which was fixed above the ultrasonic transducer of a KS-2200DB ultrasonic cleaning bath (Kunshan Jielimei, China). The equipment was operated at a constant power of 75 W and a frequency of 40 kHz. The reaction system was maintained at ambient temperature using an ice-water bath, and the water level of the bath was kept consistent with the liquid level inside the reaction tube. 5 mg of sample was dispersed into 20 mL of deionized water. The resulting mixture was then treated with ultrasonic vibration to initiate the catalytic reaction. Aliquots of the reaction solution were withdrawn at predetermined time intervals and filtered for subsequent testing.

3. Results and discussion

3.1. Structure and morphology analysis

The donor-acceptor (D-A) polymers were synthesized via a facile one-pot thermal polycondensation of melamine (electron donor) and terephthalic acid (electron acceptor), as schematically illustrated in **Figure 1a**. Two polymer samples designated MTP-*x* (*x* = 120 and 150) were synthesized by varying the polycondensation temperature [15]. The SEM images of MTP-*x* (**Figure 1b** and **Figure S1**) reveal an irregular bulk morphology formed by the aggregation of nanoscale primary particles, with no well-defined faceted crystalline grains observed. The inset TEM image further corroborates the amorphous nature of the polymer, with no long-range-ordered lattice fringes detected [16]. Consistent with the TEM observation, the XRD profiles (**Figure S2**) of both MTP-120 and MTP-150 exhibit only a broad diffraction peak across the 2θ range of 10° to 80°, which confirms the extremely low crystallinity and amorphous nature of the as-prepared D-A polymers [17].

The surface chemical composition and elemental bonding configurations of the MTP polymers were characterized by XPS. The full survey spectra (**Figure S3a**) confirmed the presence of C, N, and O elements in both polymer samples, aligning perfectly with the theoretical composition predicted for the designed D-A polymer framework [18]. Deconvolution of the high-resolution C 1s spectra revealed three distinct peaks, which were attributed to the C-C bond, the amide

C=O moiety, and the N-C=N species of the triazine ring (**Figure S3b**) [19,20]. Meanwhile, the high-resolution O 1s spectra were resolved into two peaks assigned to C=O and C-O groups (**Figure S3c**) [21]. Furthermore, analysis of the high-resolution N 1s spectra (**Figure 1c**) provided deeper insight into the nitrogen chemical environment. Both MTP-120 and MTP-150 exhibit two well-resolved characteristic peaks. The peak centered at ~398.3 eV is ascribed to sp²-hybridized nitrogen in the C-N=C moiety of the triazine ring from the MA units [22], while the peak at ~399.5 eV is assigned to C-NH_x species originating from the newly formed amide linkages and unreacted terminal amino groups [23]. These XPS results confirm that the triazine skeleton of the MA monomer is well retained during the polycondensation process, and that the amidation reaction between amino and carboxyl groups is successfully realized, further verifying the reliable construction of the target D-A polymer framework [24].

To further validate the successful fabrication of the D-A polymers, Fourier-transform infrared (FTIR) spectroscopy was employed. The spectra illustrating the as-synthesized polymers and their raw monomers are presented in **Figure 1d**. In contrast to the spectral profiles of the MA and TPA precursors, the MTP polymers exhibit markedly distinct characteristic vibrational peaks. The characteristic stretching vibration peaks of primary amino groups (-NH₂) from melamine (MA) within the 3100-3500 cm⁻¹ range, along with the C-O stretching mode of carboxyl groups from TPA at ~1285 cm⁻¹, are significantly attenuated in the FTIR spectra of both MTP-120 and MTP-150 [25]. Meanwhile, the characteristic vibrational bands of the cyanuric ring (~1543 cm⁻¹) and amide C=O (~1689 cm⁻¹) remain intact within the polymer matrix [23]. These FTIR observations for MTP-120 and MTP-150 confirm the successful construction of the desired D-A polymer structures.

Raman spectroscopy was further employed to examine the local structural environments of MTP-120 and MTP-150 (**Figure 1e**). Both MTP-120 and MTP-150 exhibit characteristic bands at approximately 680 and 980 cm⁻¹, which are associated with the deformation and breathing vibrations of the triazine rings, respectively. Nevertheless, their Raman profiles show discernible differences. MTP-120 displays a larger number of relatively sharp and distinguishable bands over the 600-1700 cm⁻¹ region, whereas several of these bands are attenuated or broadened in MTP-150. These spectral differences indicate that the two polymers possess different local vibrational and bonding environments, which may originate from temperature-dependent structural evolution during polycondensation. These spectral differences indicate distinguishable local

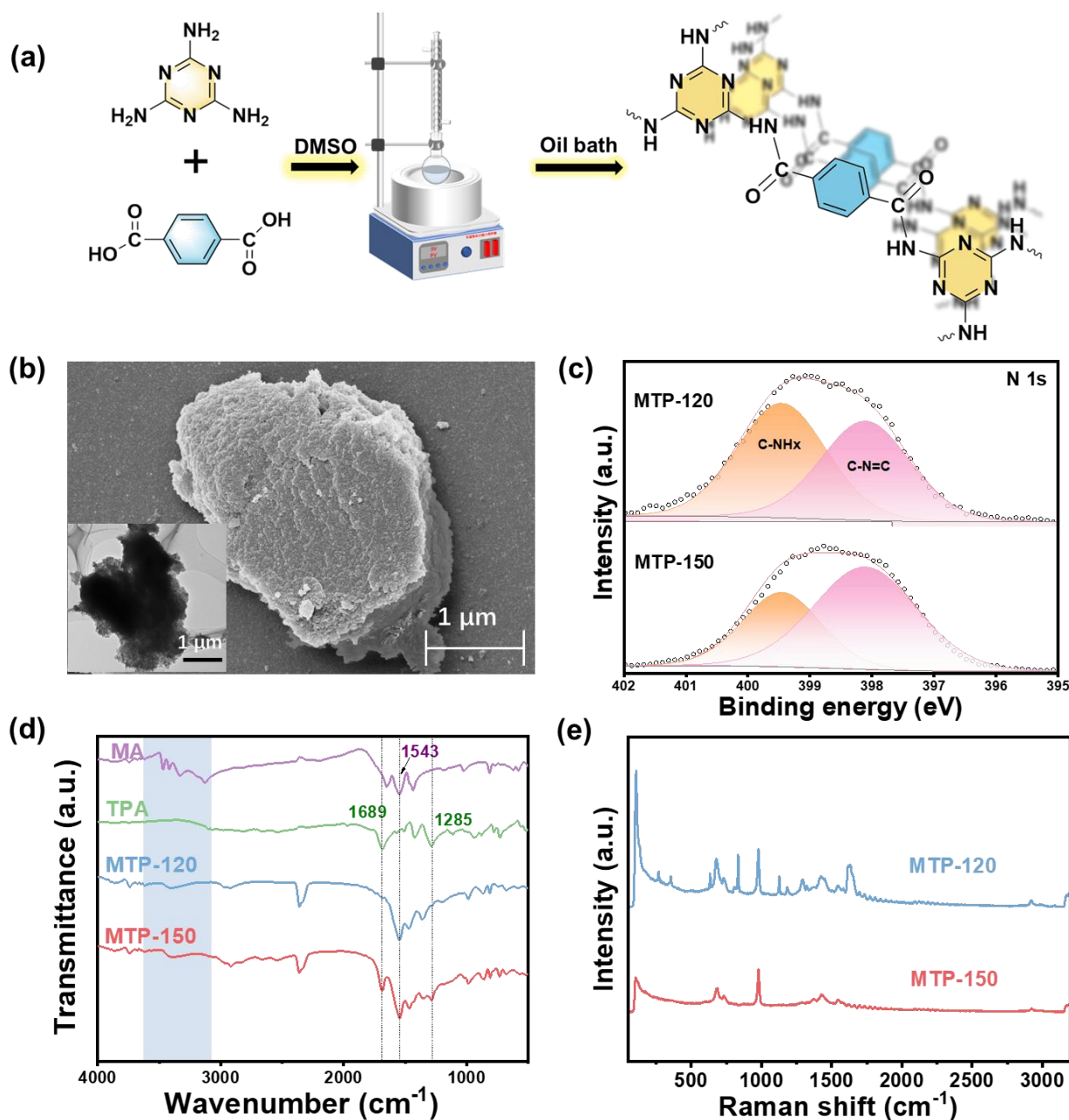


Figure 1. (a) Synthesis scheme of MTP D-A polymers from MA and TPA. (b) SEM image of MTP-150, inset: corresponding TEM image. (c) High-resolution N 1s XPS spectra of MTP-120 and MTP-150. (d) FTIR spectra of MA, TPA, MTP-120 and MTP-150. (e) Raman spectroscopy of MTP-120 and MTP-150.

bonding and vibrational environments in the two polymers, suggesting that the polycondensation temperature affects the local organization of the polymer framework.

3.2. Energy band structure analysis

To validate the D-A alternating structure in the as-

prepared MTP polymers, we first carried out density functional theory (DFT) calculations to visualize the spatial distribution of frontier molecular orbitals. As shown in **Figure 2a**, the highest occupied molecular orbital (HOMO) electron cloud is predominantly localized on the electron-rich triazine ring of the melamine donor unit, whereas the lowest unoccupied

molecular orbital (LUMO) electron density is fully delocalized on the electron-deficient benzene ring of the terephthalic acid acceptor unit. This complete spatial separation of HOMO and LUMO not only confirms the successful fabrication of the target D-A structure, but also indicates that the intramolecular charge transfer effect can be effectively triggered within the polymer backbone, facilitating the separation of piezoelectrically generated charge carriers^[14]. Building on the electronic structure insights from DFT calculations, we proceeded to evaluate the band gap, semiconductor properties and energy level alignment of the MTP polymers through UV-Vis diffuse reflectance spectroscopy (DRS) (**Figure S4**) and Mott-Schottky measurements. Based on the Tauc plots (**Figure 2b**), the calculated band gaps (E_g) for MTP-120 and MTP-150 were determined to be 3.65 eV and 4.24 eV, respectively. The wide band gap of the MTP polymers ensures a strong redox capacity of the piezoelectrically generated free charge carriers, while the ultrasonic-induced piezoelectric potential can effectively drive the separation and transport of these free carriers to the catalyst surface to participate in subsequent redox processes. Electrochemical characterization via Mott-Schottky (M-S) analysis (**Figure 2c-d**) revealed that both MTP-120 and MTP-150 are typical n-type semiconductors, with flat band potentials (E_{fb}) recorded at -1.69 V and -1.34 V vs. RHE, respectively. Typically, in an n-type semiconductor, its conduction band minimum (CBM) is approximately 0.1–0.2 V more negative than the flat band potential^[26]. The CBMs of MTP-120 and MTP-150 are located at -1.79 V and -1.44 V vs. RHE, respectively, while their valence band maxima (VBM) are located at 1.86 V and 2.8 V vs. RHE. The complete energy band alignment of the MTP polymers, along with the standard redox potentials for H_2O_2 generation, is summarized in **Figure 2e**. From the perspective of thermodynamics, the CBM potentials of both polymers are significantly more negative than the redox potential of $O_2/\bullet O_2^-$ (-0.33 V vs. RHE), which means the piezoelectrically generated free electrons have sufficient reduction capacity to reduce dissolved O_2 to superoxide radicals or H_2O_2 ^[27].

3.3. Piezoelectric properties analysis

The intrinsic piezoelectric properties of the as-prepared polymers were comprehensively investigated using piezoresponse force microscopy (PFM). Both MTP-120 and MTP-150 exhibit the classic

characteristics of piezoelectric materials, including well-defined butterfly-shaped amplitude-voltage curves and a nearly 180° phase flip in the phase-voltage hysteresis loops (**Figure 3a-b**)^[28]. These results confirm that both polymers possess intrinsic switchable polarization and piezoelectric response, which is the prerequisite for generating built-in piezoelectric potential to drive carrier generation and separation under ultrasonic vibration^[29]. Notably, MTP-150 exhibits a remarkably larger vibration amplitude than MTP-120 under an identical applied bias. The effective piezoelectric coefficient d_{33} was calculated from the amplitude-voltage curves via the formula $d_{33} = (D - D_1)/(V - V_1)$, where D_1 and V_1 represent the displacement and voltage at the intersection of the butterfly loop, while D and V correspond to the displacement and voltage at arbitrary points along the loop^[8]. The maximum effective d_{33} of MTP-150 reaches 5.02 pm/V, which is significantly larger than that of MTP-120 (1.94 pm/V). The stronger piezoelectric response enables MTP-150 to generate a higher built-in piezoelectric potential under ultrasonic excitation, which can effectively separate the piezoelectrically induced free charges to suppress their recombination.

The separation efficiency of piezoelectrically generated free charges was directly evaluated via transient piezocurrent measurements under periodic on-off ultrasonic excitation (**Figure 3c**). Both MTP-120 and MTP-150 deliver rapid and reversible piezocurrent responses with excellent repeatability over multiple ultrasonic on-off cycles, confirming the stable piezoelectric excitation of free charges in the polymer^[11]. Remarkably, the steady-state piezocurrent intensity of MTP-150 is nearly 3 times that of MTP-120. This significant enhancement highlights the superior charge separation efficiency of MTP-150, corroborating the earlier PFM findings. Furthermore, electrochemical impedance spectroscopy (EIS) was utilized to probe the interfacial charge transfer dynamics. As shown in the Nyquist plots (**Figure 3d**), the diameter of the semicircle in the high-frequency region represents the charge transfer resistance (R_{ct}). MTP-150 exhibits a significantly smaller semicircle diameter than MTP-120, indicating a much lower R_{ct} and a faster interfacial charge transfer process^[30]. The accelerated charge transfer kinetics can effectively reduce the recombination probability of free carriers during their migration to the catalyst surface, thus maximizing the utilization of active charge carriers for H_2O_2 generation.

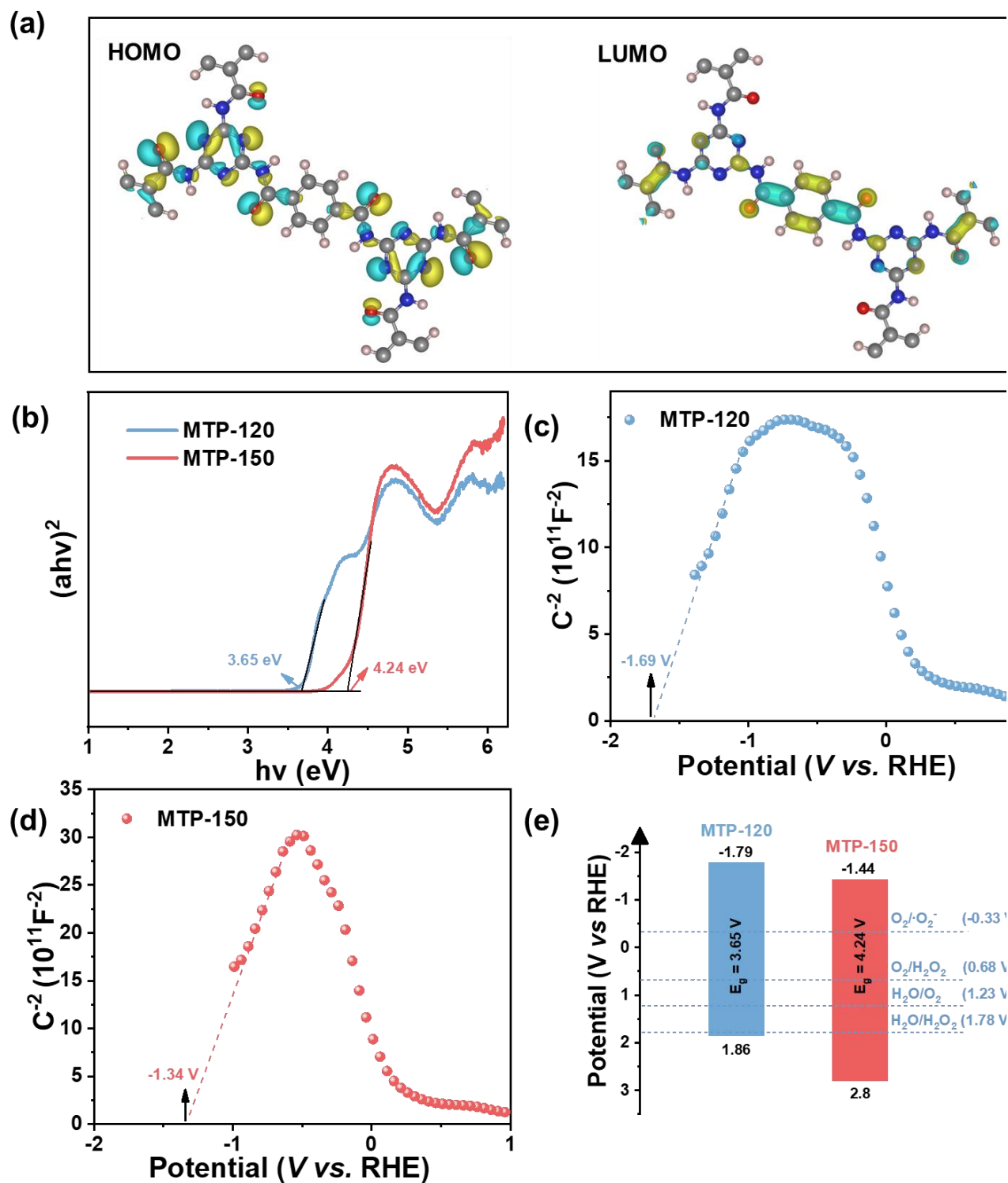


Figure 2. (a) Spatial distributions of the HOMO and LUMO of the D-A polymer. (b) Tauc plots derived from UV-Vis DRS for MTP-120 and MTP-150. Mott-Schottky profiles of (c) MTP-120 and (d) MTP-150. (e) Energy band alignment diagrams of MTP-120 and MTP-150, together with the standard redox potentials for H_2O_2 generation.

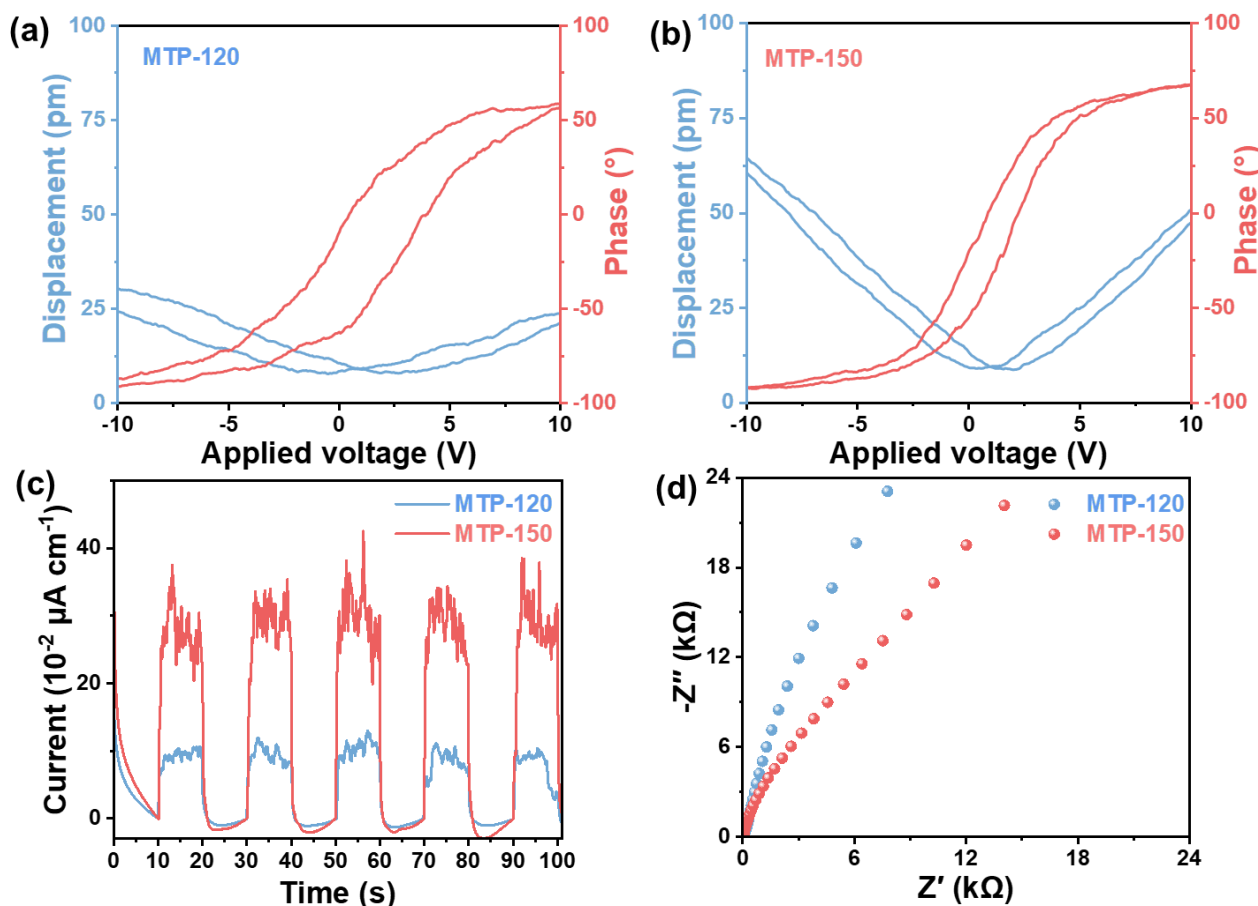


Figure 3. PFM amplitude-voltage butterfly curves (blue) and corresponding phase hysteresis loops (red) for (a) MTP-120 and (b) MTP-150. (c) Time-dependent piezocurrent responses and (d) EIS Nyquist plots of polymers.

3.4. Piezoelectric H_2O_2 generation

The piezocatalytic H_2O_2 generation activity of the as-synthesized polymers was assessed under ultrasonic vibration. The piezocatalytic H_2O_2 production over MTP-150 increases almost linearly with ultrasonic irradiation time, achieving a generation rate of 4.3 mmol g^{-1} in 30 min (**Figure 4a**). In sharp contrast, only a trace amount of H_2O_2 was produced after 30 min of ultrasonic irradiation in the absence of the catalyst, or under mechanical stirring without ultrasonic vibration, confirming that the observed H_2O_2 generation is dominated by the piezocatalytic activity of MTP-150 rather than sonochemical effects from ultrasonic cavitation (**Figure S5**). MTP-120 exhibits negligible H_2O_2 production activity under the same reaction conditions, demonstrating the superior piezocatalytic performance of MTP-150. This significant performance

difference is primarily associated with the enhanced piezoelectric response, improved charge separation efficiency, and accelerated interfacial charge transfer kinetics of MTP-150, which provide more active charge carriers for the catalytic redox reactions to generate H_2O_2 . In addition, the H_2O_2 production capacity of MTP-150 remains almost unchanged after five consecutive reaction cycles, demonstrating its remarkable structural integrity and catalytic recyclability (**Figure 4b**). To further evaluate the structural stability of MTP-150, the catalyst recovered after five consecutive piezocatalytic cycles was characterized by XRD, FTIR, and XPS (**Figure S6**). The used sample retains the broad XRD feature of the fresh MTP-150 without the emergence of additional crystalline phases. Moreover, the characteristic FTIR bands associated with the triazine framework and amide linkages remain essentially unchanged. Quantitative

XPS analysis reveals moderate variations in the surface elemental composition after cycling, with the C/N atomic ratio changing from 1.67 to 1.39 and the O content increasing from 4.37 to 6.95 at.% (Table S1). Nevertheless, the major chemical states of C, N, and O remain largely preserved, without the appearance of pronounced new chemical states. These results confirm that the principal polymer framework and surface chemical structure of MTP-150 are largely preserved during repeated piezocatalytic reactions. Remarkably,

the H_2O_2 production rate obtained in this study outperforms the majority of previously reported piezoelectric catalysts, including classical perovskite oxides, bismuth-based materials, carbon nitride-based composites, and other polymer-based catalysts (Figure 4c and Table S2) [5, 31–43]. This outstanding performance confirms that rational construction of the D-A alternating structure is an effective strategy to develop high-efficiency polymer piezoelectric catalysts for H_2O_2 production.

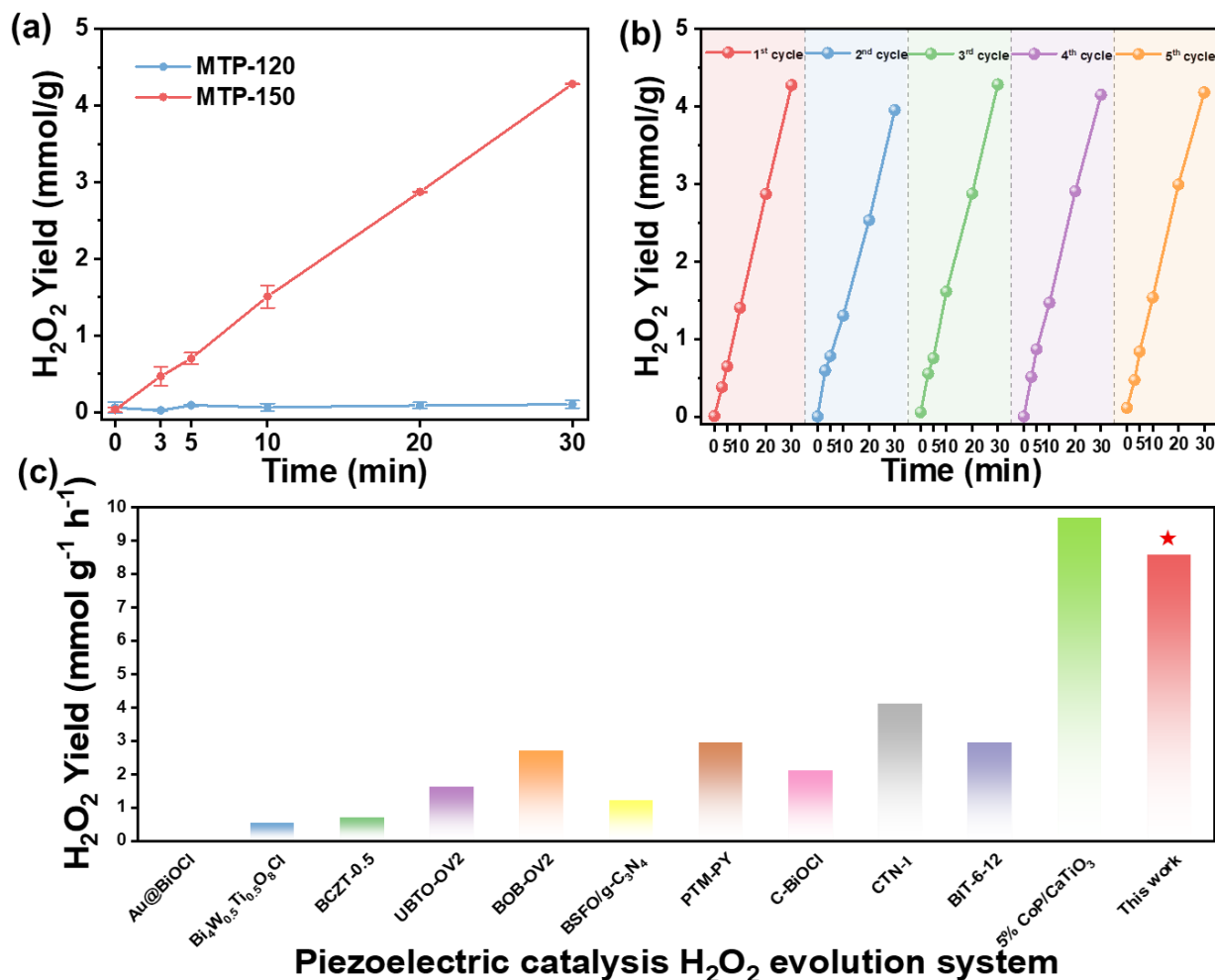


Figure 4. (a) Time-resolved piezocatalytic H_2O_2 generation profiles of MTP-120 and MTP-150 under ultrasonic irradiation. (b) Cycling stability test of piezocatalytic H_2O_2 production over MTP-150 for five consecutive cycles. (c) Comparison of piezocatalytic H_2O_2 production rates between MTP-150 and recently reported piezocatalysts. Detailed experimental parameters are available in Table S1 (Supporting Information).

To reveal the underlying reaction mechanism of piezocatalytic H_2O_2 production, radical quenching tests were carried out to pinpoint the dominant reactive species involved in the piezoelectric H_2O_2 formation

(Figure 5a). p-benzoquinone (p-BQ), sodium iodate (NaIO_3) and tert-butanol (TBA) were introduced as selective quenchers for superoxide radicals ($\cdot\text{O}_2^-$), piezoelectrically induced free electrons, and hydroxyl

radicals ($\bullet\text{OH}$), respectively. The H_2O_2 production was strongly suppressed in the presence of either p-BQ or NaIO_3 . Because p-BQ can quench superoxide-related intermediates while also accepting electrons, its inhibitory effect alone cannot be regarded as exclusive evidence for $\bullet\text{O}_2^-$. Nevertheless, the simultaneous inhibition by p-BQ and the electron scavenger NaIO_3 indicates that piezoinduced electrons and the subsequent O_2 reduction process play central roles in H_2O_2 formation. In contrast, TBA caused only a marginal decrease in the H_2O_2 yield, suggesting a limited contribution from $\bullet\text{OH}$.^[44] This finding is also corroborated by the band structure analysis, where the sufficiently negative conduction band potential of MTP-150 provides a strong thermodynamic driving force to convert dissolved O_2 to $\bullet\text{O}_2^-$ radicals. To provide direct spectroscopic evidence for the generation of these active radicals under piezoelectric excitation, we performed electron paramagnetic resonance (EPR) measurements with DMPO as the spin-trapping agent. As displayed in **Figure 5b** and **Figure S7**, the typical characteristic peaks of DMPO- $\bullet\text{O}_2^-$ and DMPO- $\bullet\text{OH}$ adducts can be collected and their intensities increase gradually with prolonged ultrasonic irradiation time. This observation offers direct spectroscopic confirmation of the sustained formation of $\bullet\text{O}_2^-$ and $\bullet\text{OH}$ radicals under piezoelectric excitation^[8]. Atmosphere control experiments (**Figure 5c**) show that only a negligible amount of H_2O_2 is detected in the N_2 -saturated reaction system with no dissolved oxygen, while markedly enhanced H_2O_2 production is observed in the air-saturated system, with a further significant increase under O_2 -saturated conditions. This stark contrast confirms that dissolved oxygen is an indispensable reactant for H_2O_2 formation, and the piezocatalytic H_2O_2 production over MTP-150 is dominated by the two-electron ORR pathway, rather than the water oxidation pathway^[5]. Given the pivotal contribution of dissolved oxygen and the ORR mechanism to H_2O_2 formation, oxygen temperature programmed desorption (O_2 -TPD) measurements were performed, and the results (**Figure 5d**) directly visualize the difference in this critical property between the two polymers. MTP-150 exhibits a much stronger and broader oxygen desorption peak with a substantially larger integrated peak area than MTP-120, demonstrating its enhanced capability to adsorb and activate oxygen molecules. This strengthened oxygen adsorption enriches a high density of reactant molecules on the catalyst surface, while also promoting the stabilization and further activation of $\bullet\text{O}_2^-$ key intermediates, collectively accelerating the two-electron ORR kinetics for efficient H_2O_2 production^[45].

3.5. Theoretical calculations and mechanistic insights

To elucidate the atomic-level structure-property relationships underlying the piezocatalytic H_2O_2 production, density functional theory (DFT) calculations were carried out. The electron localization function (ELF) map in **Figure 6a** visualizes the spatial distribution of electrons in the polymer framework. A high degree of electron delocalization is clearly observed along the entire conjugated polymer backbone, which provides a continuous, low-resistance pathway for the transport of piezoelectrically generated free electrons^[46]. We further systematically evaluated the adsorption behavior of O_2 on the D-A polymer surface. After screening all possible adsorption sites and comparing the corresponding adsorption energies (**Figure S8** and **Figure S9**), we identified the benzene ring moiety as the most thermodynamically favorable O_2 adsorption site, as shown in **Figure 6b**. Remarkably, this optimal adsorption site coincides exactly with the LUMO distribution of the D-A polymer, as revealed in our earlier frontier molecular orbital calculations. This spatial matching effectively shortens the electron transfer pathway between the catalyst and adsorbed O_2 , minimizing charge recombination during the transfer process^[47]. Under normal conditions, the DFT-calculated O_2 adsorption energy is -0.25 eV, which is characteristic of a stable physical adsorption state, in good agreement with our O_2 -TPD. Upon applying mechanical strain to mimic the piezoelectric response induced by ultrasonic excitation, the adsorption energy becomes significantly more negative to -0.87 eV, indicating a dramatic enhancement in the adsorption affinity of the D-A polymer toward O_2 . Further electronic structure calculations show a net electron transfer of $0.94 e^-$ from the polymer framework to the adsorbed O_2 molecule, accompanied by a significant elongation of the O-O bond length from 1.23 Å for free O_2 to 1.51 Å after adsorption. These results provide direct evidence for strong electronic coupling between the D-A polymer and O_2 , and confirm the effective activation of the adsorbed O_2 molecule. The adsorption behavior of H_2O was also investigated. As illustrated in **Figure 6c** and **Figure S10**, H_2O preferentially adsorbs near the electron-rich triazine ring of the D-A polymer, a region that corresponds to the HOMO distribution of the framework, making it susceptible to oxidation to form protons^[48]. The adsorption energy of H_2O is calculated to be -0.80 eV under normal conditions, and it becomes more negative, reaching -1.43 eV under applied mechanical stress, demonstrating that

piezoelectric excitation also strengthens the adsorption and activation of H_2O at the polymer surface. To simulate the realistic reaction conditions during catalysis, we also performed co-adsorption calculations

for O_2 and H_2O . The co-adsorption energy is -0.42 eV under normal conditions, and it reaches -1.61 eV under 0.5 GPa hydrostatic pressure. This significant

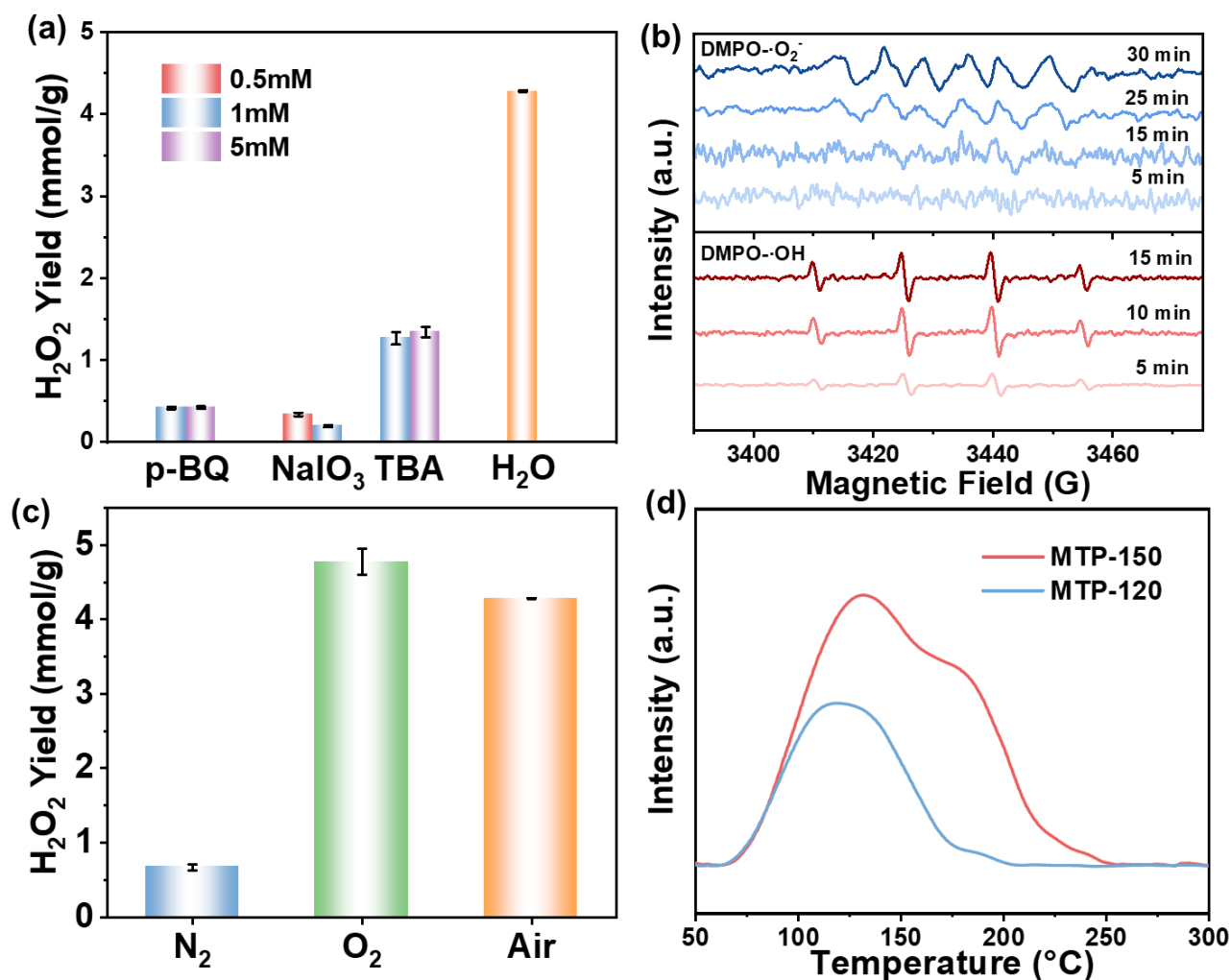


Figure 5. (a) Piezocatalytic H_2O_2 production over MTP-150 in the presence of different radical scavengers. (b) EPR spectra of DMPO- $\cdot\text{O}_2^-$ (top) and DMPO- $\cdot\text{OH}$ (bottom) recorded under ultrasonic irradiation. (c) Piezocatalytic H_2O_2 production over MTP-150 under different gas environments (N_2 , O_2 and air). (d) O_2 -TPD profiles of MTP-120 and MTP-150.

enhancement in co-adsorption affinity confirms that both reactants can be stably co-adsorbed and activated on the D-A polymer surface under piezoelectric excitation (Figure 6d). Finally, we constructed the free energy diagram of the two-electron ORR pathway for H_2O_2 generation to evaluate the effect of mechanical stress on the reaction thermodynamics, as presented in Figure 6e. Under ambient pressure, the initial adsorption of O_2 to form the $^*\text{O}_2$ intermediate is a thermodynamically uphill process with a positive free

energy change, indicating that this step is non-spontaneous and acts as the initial thermodynamic bottleneck of the reaction. When mechanical pressure is applied to simulate the piezoelectric strain induced by ultrasonic vibration, the initial O_2 adsorption step is converted into a thermodynamically downhill, spontaneous process with a significantly negative free energy change. This spontaneous adsorption eliminates the initial thermodynamic bottleneck, and greatly promotes the enrichment and activation of O_2 molecules

at the catalyst surface. Meanwhile, the free energy of the rate-determining $^*\text{OOH}$ intermediate is also drastically reduced under pressure, which further optimizes the thermodynamics of the proton-coupled electron transfer process for H_2O_2 formation. However, the substantially

lower free energy of the final $^*\text{H}_2\text{O}_2$ intermediate under pressure makes it less favorable for H_2O_2 desorption (Figure S11). Remarkably, the piezocatalytic process is driven by continuous, periodic ultrasonic vibration, which imposes cyclic, reversible mechanical strain on

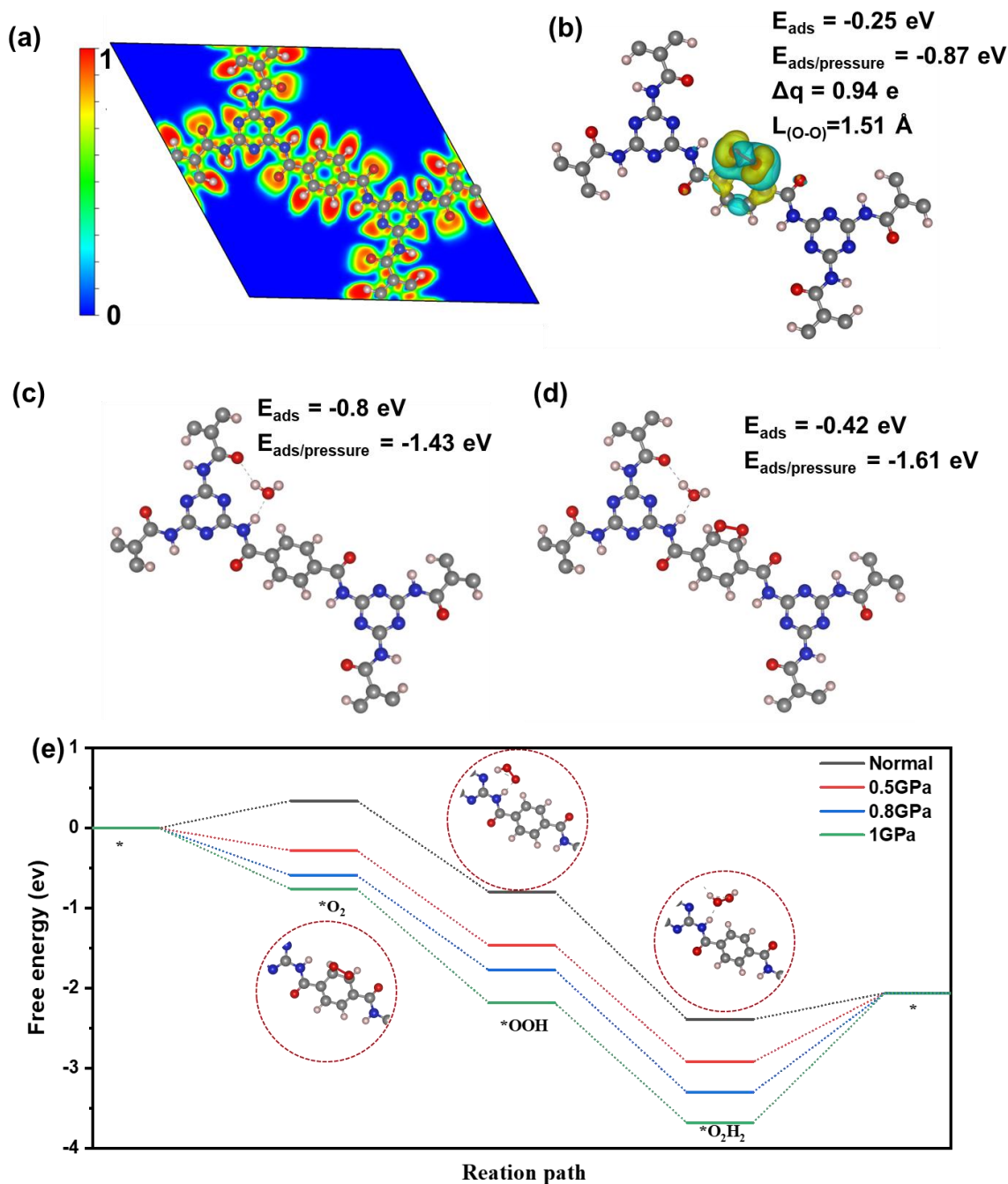


Figure 6. (a) Two-dimensional ELF map of the MTP polymer. DFT-optimized adsorption configurations of (b) O_2 , (c) H_2O , and (d) co-adsorbed O_2 and H_2O on the MTP polymer surface. (e) Gibbs free energy diagrams for the 2e^- ORR to produce H_2O_2 over the MTP polymer under normal and piezoelectric-induced pressure conditions.

the D-A polymer framework. This means the catalyst dynamically alternates between the strained (pressurized) and strain-released (ambient pressure) states throughout the reaction, rather than remaining in a static pressurized state ^[49]. Therefore, the subsequent strain-released state restores the favorable thermodynamics for rapid H₂O₂ desorption and active site regeneration. This unique synergistic effect of pressure-promoted reactant activation and decompression-promoted product desorption, enabled by the periodic piezoelectric strain, is a key factor underlying the excellent piezocatalytic H₂O₂ production performance of the D-A polymers ^[50].

Combining all the experimental characterizations and DFT calculation results, we herein elucidate the underlying piezocatalytic mechanism for H₂O₂ production over the D-A conjugated polymer, as

visually presented in **Figure 7**. Under periodic mechanical deformation induced by ultrasonic vibration, the D-A polymer triggers its intrinsic piezoelectric effect and generates a built-in piezoelectric field, which drives the efficient separation of piezoelectrically generated free charges. In the process, water molecules preferentially adsorb at HOMO-proximal triazine sites and are oxidized by free holes to generate protons, while O₂ adsorbs at LUMO-localized benzene sites, accepts free electrons to form •O₂^{•-} intermediates, and is finally converted to H₂O₂ via a two-electron ORR process ^[44]. Notably, the periodic mechanical strain dynamically alternates the polymer between pressurized and relaxed states, which synergistically facilitates O₂ activation under pressure and H₂O₂ desorption in the relaxed state, collectively boosting the overall catalytic efficiency ^[8].

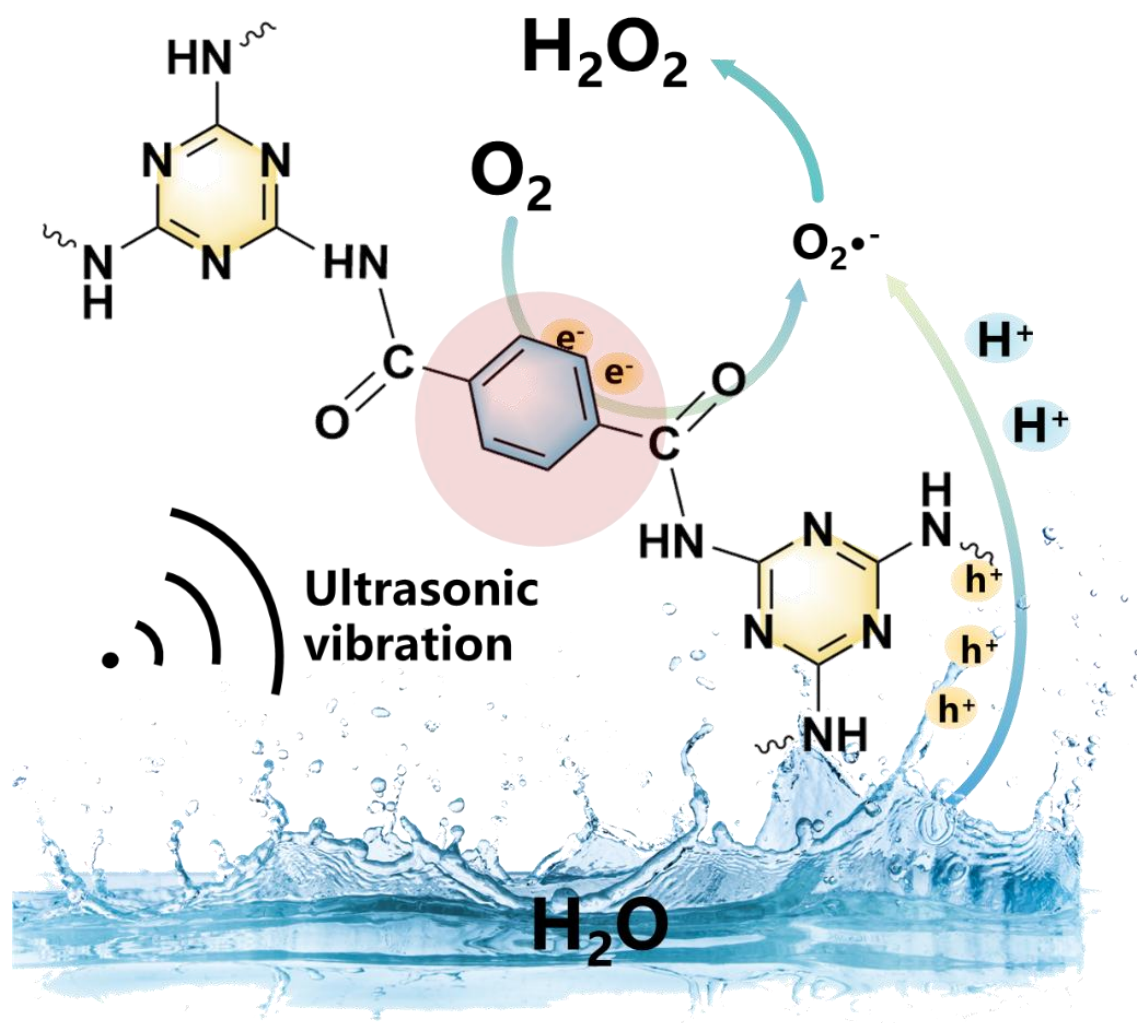


Figure 7. Schematic illustration of the piezocatalytic H₂O₂ production mechanism over the MTP D-A polymer under ultrasonic irradiation.

4. Conclusion

In this work, donor-acceptor (D-A) conjugated polymers were successfully synthesized via a facile polycondensation approach, and their application in piezocatalytic H_2O_2 production was systematically explored. The optimized polymer sample exhibits a high effective piezoelectric coefficient d_{33} , excellent piezocatalytic H_2O_2 production activity, and outstanding long-term cycling stability. Experiments and theoretical calculations reveal that the piezocatalytic H_2O_2 production over the D-A polymer follows a two-electron ORR mechanism, with piezoelectrically generated electrons and $\cdot\text{O}_2^-$ as the primary active species. The spatially separated frontier molecular orbitals of the D-A structure not only suppress charge recombination, but also provide matched independent active sites suited for the oxidation and reduction half-reactions. Meanwhile, periodic mechanical strain induced by ultrasonic vibration synergistically promotes the adsorption and activation of reactants under pressure, as well as the release of reaction products during decompression. These findings highlight the promising application prospects of D-A conjugated polymers in piezocatalysis research.

CRedit authorship contribution statement

Chenyang Liu: Writing-original draft, Methodology, Data curation, Visualization, Investigation. **Zicong Jiang:** Writing-review & editing, Supervision, Funding acquisition. **Mingshan Zhu:** Writing-review & editing, Supervision, Conceptualization

Data Availability Statement

The data that has been used is confidential.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this article. Mingshan Zhu is an editorial board member of this journal and was not involved in the editorial review or the decision to publish this article.

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