Electronic Supplementary Information

Electrocatalytic reforming of waste plastics to high value-added chemicals and hydrogen fuel

Rui Shi,†[a] Ke-Sheng Liu,†[a,b] Fulai Liu,[a] Xiao Yang,[a] Chun-Chao Hou[a] and Yong Chen*[a,b]

[a] *Key Laboratory of Photochemical Conversion and Optoelectronic Materials & HKU-CAS Joint Laboratory on New Materials, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, People's Republic of China. E-mail: chenyong@mail.ipc.ac.cn*
[b] *University of Chinese Academy of Sciences, Beijing 100049, People's Republic of China.*

Materials

All materials were of analytical grade and used as received without further purification. Ni foam (10 cm × 10 cm) was purchased from KUNSHAN JIAYISHENG ELECTRONIC CO., LTD. Platinum foil was bought from Tianjin AIDA Hengsheng Science-Technology Development Co., Ltd. Palladium chloride ($PdCl_2$), potassium hydroxide (KOH), hydrochloric acid (HCl), polyethylene terephthalate (PET), ethylene glycol (EG), glyoxal, and potassium carbonate, D_2O, and dimethyl sulfoxide (DMSO) were obtained from Sinopharm Chemcial Reagent Co., Ltd (Shanghai, China). The plastic water bottle was purchased from HuaLian supermarket, dried and ground using a grinder into pieces ≤ 01 cm^2.

Preparation of Pd modified Ni foam electrode (Pd/NF)

Ni foam (1 cm × 2 cm) was soaked in 3 M HCl for 10 min to remover surface native oxides and cleaned by ethanol and deionized water for 3 times. Pd/NF was prepared by depositing Pd on Ni foam. Firstly, 10 mL H_2PdCl_4 solution with different concentration was added to a 20 mL flask. Then the pretreated Ni foam was soaked in H_2PdCl_4 solution under stirring for 10 min. Pd nanoparticle deposited on the surface of Ni foam through displacement reaction (Eq. 1). Finally, the as-prepared Pd/NF was taken out, washed with deionized water and ethanol for three times, dried in air for 12 h. All the above operations were carried out under room temperature.

$[PdCl_4]^{2-} + Ni = Pd + Ni^{2+} + 4Cl^-$ Eq. 1

PET and real-world plastic bottle pretreatment.

2 g PET was pretreated in 60 mL of 10 M KOH solution at 60 °C for 3h, and the resulting suspension was used as the electroreforming substrate in a three-electrode system. 0.5 g real-world plastic bottle was pretreated in 60 mL of 10 M KOH solution at 60 °C for 3 h, and the resulting suspension was used as electroreforming substrate in a two-electrode system.

Materials characterization

The purity and crystallinity of the as-prepared sample were characterized by XRD on a Bruker D8-advance diffractometer using Cu Kα (λ=1.54056 Å). The XRD data for indexing and cell-parameter calculation were collected in a scanning mode with a step length of 0.1° and a preset time of 1s/step. Morphologies of the as-prepared sample were examined by Hitachi S-4800 field emission scanning electron microscope (SEM). Chemical characterization of the sample surface was performed with X-ray photoelectron spectroscopy (XPS ThermoFisher ESCALAB 250Xi). The charge effect was calibrated using the binding energy of C1s. Morphologies and structures of the as-prepared sample were examined with high resolution transmission electron microscopy (HRTEM) by JEM 2100F field emission gun transmission electron microscope operated at an accelerating voltage of 200 kV. Elemental analysis data of samples were obtained using inductively coupled plasma atomic emission spectrometry (ICP-OES Varian 710-OES, USA). The quantities of H_2 evolution were measured by a gas chromatograph (GC-2014C, Shimadzu, with Ar as carrier gas), which was equipped with a 5 Å molecular sieve column (3 m × 2 mm) and a thermal-conductivity detector.

Electrochemical measurements.

A standard three-electrode system on CHI660 electrochemical workstation was employed to examine all the electrochemical measurements except for special instructions. H-type cell separated by proton exchange membrane was used. Pt foil was used as the counter electrode for HER. Hg/HgO was used as the reference electrode, which was calibrated by reversible hydrogen electrode (RHE): $E(RHE) = E(Hg/HgO) + 0.059 \times pH + 0.098$. Pd/NF was used as the working electrode, and the actual area immersed in the electrolyte was 1 cm × 1 cm. The current density was calculated using the geometrical surface of 1 cm^2. The experiments were conducted in 60 mL of KOH electrolyte. The electrocatalytic activity of Pd/NF for EG oxidation was investigated with CV method in KOH solution at a scan rate of 10 mVs^{-1}. PET electroreforming was carried out at a potentiostatic mode. During the electroreforming process, the concentrations of products were quantified by ^{1}H-NMR and ^{13}C-NMR spectroscopy. ^{1}H-NMR and ^{13}C-NMR spectroscopies were collected on a 700 MHz Bruker spectrometer. All NMR sample preparation is as follows: 300 μL product electrolyte + 300 μL D_2O + 30 μL DMSO (internal standard). The quantity of products in the samples was calculated by Eq.2

$$m_{product} = \frac{I_{product} \times N_{DMSO} \times M_{product}}{I_{DMSO} \times N_{product} \times M_{DMSO}} \times m_{DMSO} \times n \qquad \text{Eq. 2}$$

where $I_{product}$ is the integral of product peak; $N_{product}$ is the numbers of proton or carbon corresponding to product peak; $M_{product}$ is the molar mass of product; m_{DMSO} is the mass of DMSO; n = 60 mL/300 μL = 200.

The faradaic efficiency for PET electroreforming was defined as the quantity of electric charges used for producing carbonate divided by the total charge passing through the electrodes during the electrolysis. Five electrons are needed to produce one carbonate ion, so the faradaic efficiency can be calculated by Eq. 3:

$$EF_{carbonate} = (5 \times m_{carbonate} / M_{carbonate} \times F) / Q \qquad \text{Eq. 3}$$

where $m_{carbonate}$ is the mass of potassium carbonate, $M_{carbonate}$ is molar mass of potassium carbonate, F is the faraday constant and Q is the total number of charges passing through the catalyst.

In the two-electrode system, we applied Pd/NF as the anode and Ni foam as the cathode to electroreform the real-world plastic bottle. During the electroreforming process, the concentrations of liquid products were quantified by ^{1}H-NMR and ^{13}C-NMR spectroscopy. H_2 was measured by a gas chromatograph (GC-2014C, Shimadzu, with Ar as carrier gas), which was equipped with a 5Å molecular sieve column (3 m × 2 mm) and a thermal-conductivity detector.

Table S1 The loading mass of Pd, Q value and ECSA of Pd/NF catalysts prepared in different concentrations of H_2PdCl_4 solution.

Sample	5 mM	10 mM	20 mM	30 mM
Q^a ($mC\cdot cm^{-2}$)	342.2	728.9	862.6	884.1
Loading mass[b] (mg)	5.31	10.59	21.25	31.73
ECSA ($m^2\cdot g^{-1}$)	149.8	160.1	94.4	64.8

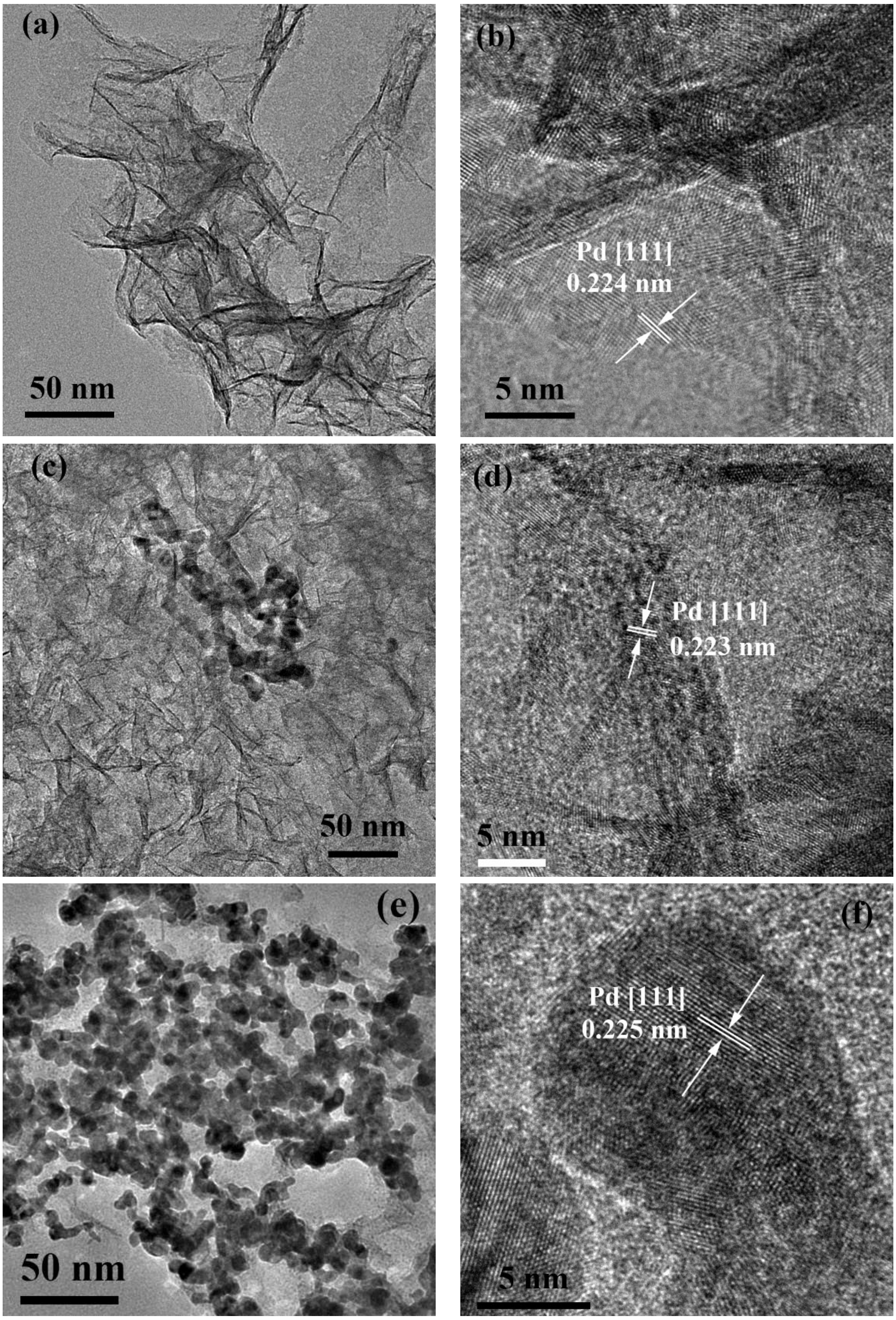
[a] Q value is the integral area of reduction wave of Pd surface oxides ranging from 0.02 to 0.65 V vs. RHE in Fig. 2a.

[b] The loading mass of Pd catalyst on NF were obtained based on the results of ICP measurement.

The electrochemical active surface area (ECSA) of Pd/NF can be calculated from the Coulombic charge for the reduction of Pd oxides using the Eq. 4:

$$\mathrm{ECSA} = Q / (0.43 \times m) \qquad \text{Eq. 4}$$

Q is the columbic charge for the reduction of Pd oxides (as shown in Table S1); 0.43 ($mC\cdot cm^{-2}$) is a constant assuming that a monolayer of Pd oxides is reduced on the Pd surface; m (mg) is the mass of Pd loading on the surface of working electrode (as shown in Table S1).[1]


(a)
50 nm
(b)
Pd [111]
0.224 nm
5 nm
(c)
50 nm
(d)
Pd [111]
0.223 nm
5 nm
(e)
50 nm
(f)
Pd [111]
0.225 nm
5 nm

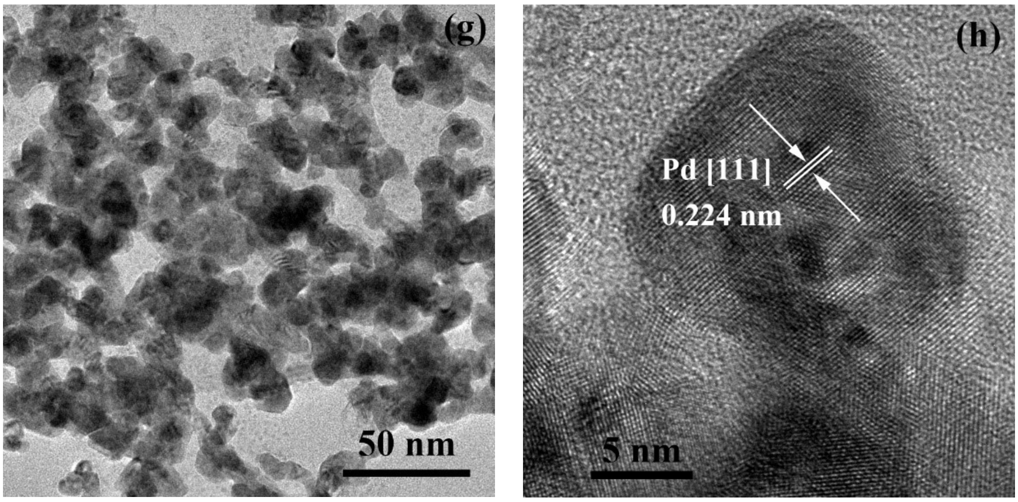


Fig. S1 TEM and HRTEM images of (a-b) Pd/NF-5, (c-d) Pd/NF-10, (e-f) Pd/NF-20, (g-h) Pd/NF-30.

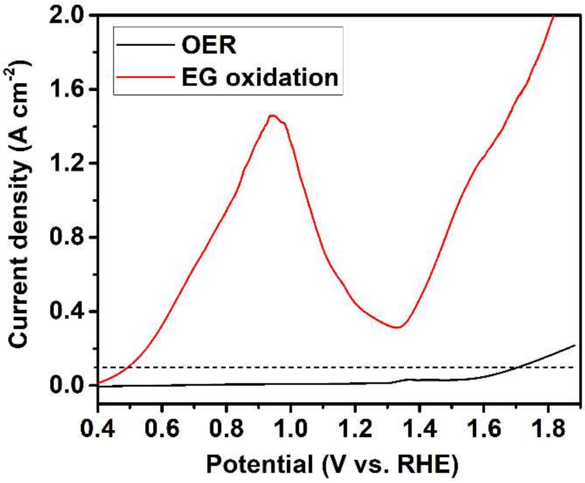


Fig. S2 LSV curves of Pd/NF-10 in 10 M KOH solution with 0.0 M EG (OER) and 1 M EG (EG oxidation) at a scan rate of 10 mV s^{-1}.

As shown in Fig. S2, Pd/NF-10 demonstrates EG electrooxidation activity with potential of 0.94 V vs. RHE to reach maximum current density of 1450 mA, while OER activity by Pd/NF-10 is very poor with high potential of 1.69 V vs RHE to reach current density of 100 mA cm^{-2}. In the potential range of EG oxidation (0.4 to 1.4 V vs RHE), OER did not occur.

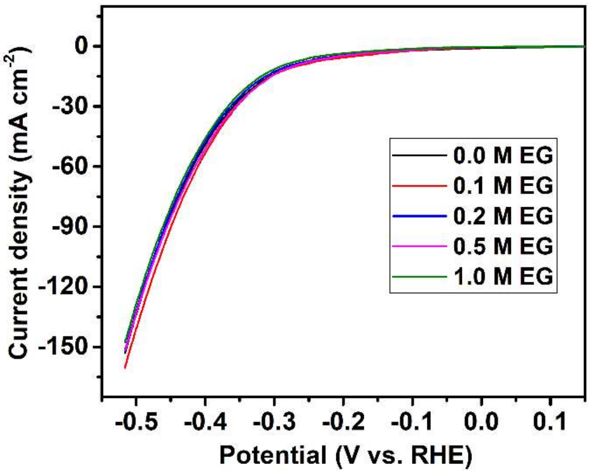


Fig. S3 LSV curves of Pt foil in 10 M KOH solution with different concentrations of EG at a scan rate of 10 mV s^{-1}.

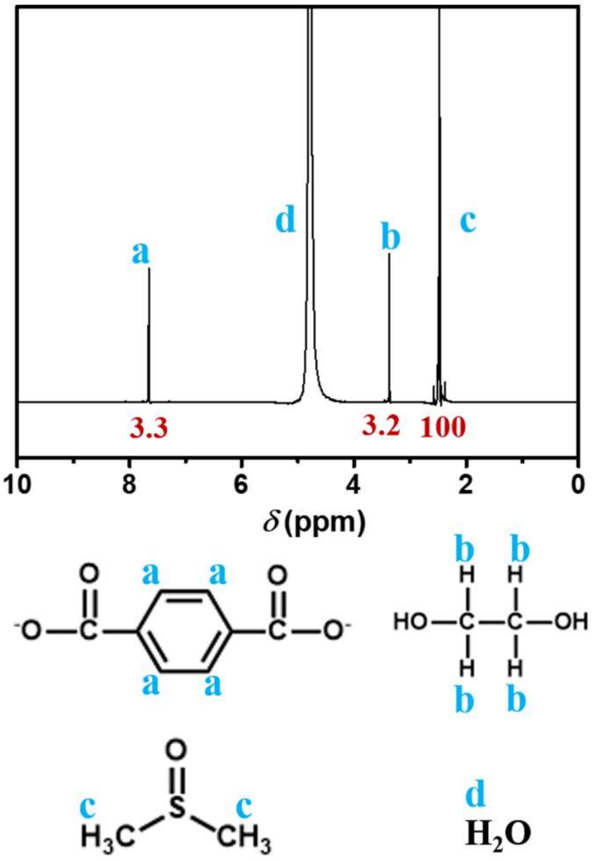


Fig. S4 ^{1}H-NMR spectrum of PET substrate after pretreated in 60 mL of 10 M KOH solution at 60 °C for 4 h.

$$m_{terephthalate} = \frac{I_{terephthalate} \times N_{DMSO} \times M_{terephthala}}{I_{DMSO} \times N_{terephthalate} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{3.3 \times 6 \times 242}{100 \times 4 \times 78} \times 33\ \mathrm{mg} \times 200 = 1013\ mg$$

$$Yield_{terephthal} = \frac{1013\ mg}{2521\ mg} \times 100\% = 40.2\ \%$$

$$m_{EG} = \frac{I_{EG} \times N_{DMSO} \times M_{EG}}{I_{DMSO} \times N_{EG} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{3.2 \times 6 \times 62}{100 \times 4 \times 78} \times 33\ \mathrm{mg} \times 200 = 252\ mg$$

$$Yield_{EG} = \frac{252\ mg}{646\ mg} \times 100\% = 39\ \%$$

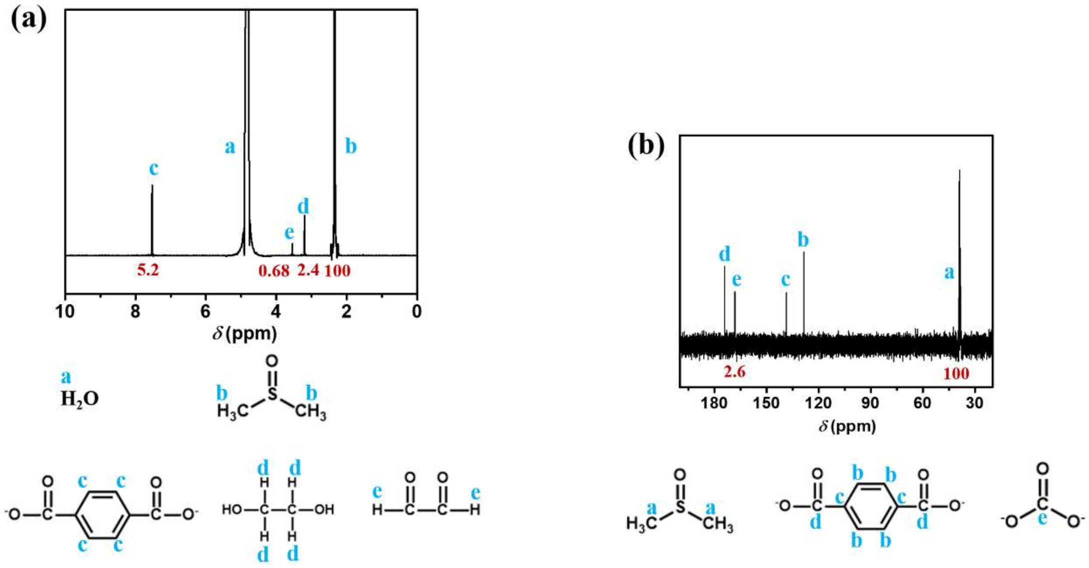


Fig. S5 (a) ^{1}H-NMR and (b) ^{13}C-NMR spectra after PET electroreforming for 5 h.

$$m_{terephthalate}=\frac{I_{terephthalate}\times N_{DMSO}\times M_{terephthalatet}}{I_{DMSO}\times N_{terephthalate}\times M_{DMSO}}\times m_{DMSO}\times n$$

$$=\frac{5.2\times 6\times 242}{100\times 4\times 78}\times 33\text{ mg}\times 200=1597\,mg$$

$$m_{EG}=\frac{I_{EG}\times N_{DMSO}\times M_{EG}}{I_{DMSO}\times N_{EG}\times M_{DMSO}}\times m_{DMSO}\times n$$

$$=\frac{2.4\times 6\times 62}{100\times 4\times 78}\times 33\text{ mg}\times 200=189\,mg$$

$$m_{glyoxal}=\frac{I_{glyoxal}\times N_{DMSO}\times M_{glyoxal}}{I_{DMSO}\times N_{glyoxal}\times M_{DMSO}}\times m_{DMSO}\times n$$

$$=\frac{0.68\times 6\times 58}{100\times 2\times 78}\times 33\text{ mg}\times 200=100.1\,mg$$

$$m_{carbonate}=\frac{I_{carbonate}\times N_{DMSO}\times M_{carbonate}}{I_{DMSO}\times N_{carbonate}\times M_{DMSO}}\times m_{DMSO}\times n$$

$$=\frac{2.6\times 2\times 138}{100\times 1\times 78}\times 33\text{ mg}\times 200=607\,mg$$

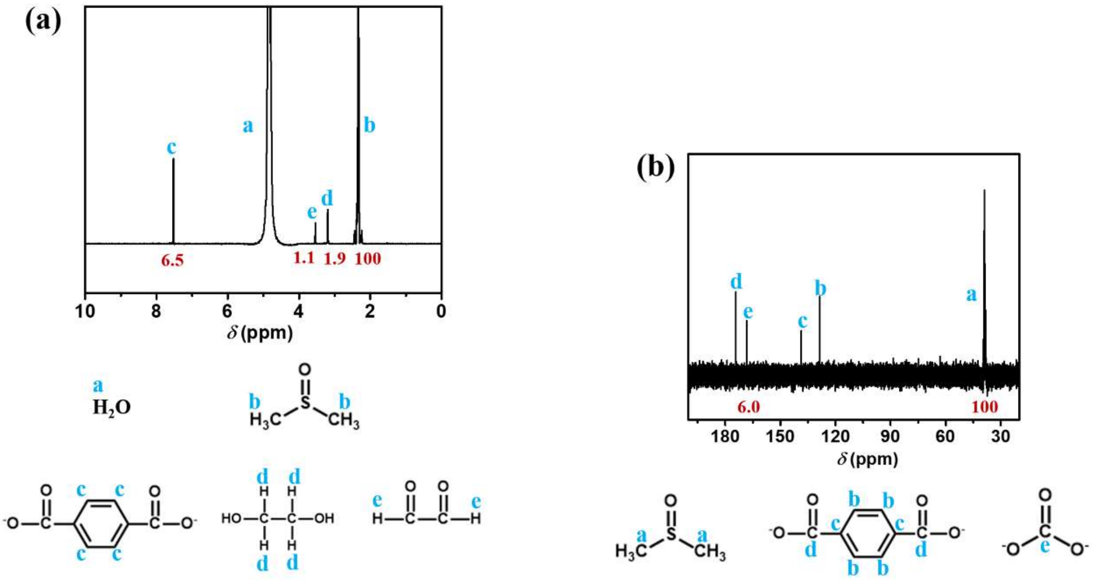


Fig. S6 (a) ^{1}H-NMR and (b) ^{13}C-NMR spectra after PET electroreforming for 10 h.

$$m_{terephthalat} = \frac{I_{terephthalat} \times N_{DMSO} \times M_{terephthalat}}{I_{DMSO} \times N_{terephthalat} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{6.5 \times 6 \times 242}{100 \times 4 \times 78} \times 33\ \mathrm{mg} \times 200 = 1997\ mg$$

$$m_{EG} = \frac{I_{EG} \times N_{DMSO} \times M_{EG}}{I_{DMSO} \times N_{EG} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{1.9 \times 6 \times 62}{100 \times 4 \times 78} \times 33\ \mathrm{mg} \times 200 = 149\ mg$$

$$m_{glyoxal} = \frac{I_{glyoxal} \times N_{DMSO} \times M_{glyoxal}}{I_{DMSO} \times N_{glyoxal} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{1.1 \times 6 \times 58}{100 \times 2 \times 78} \times 33\ \mathrm{mg} \times 200 = 162\ mg$$

$$m_{carbonate} = \frac{I_{carbonate} \times N_{DMSO} \times M_{carbonate}}{I_{DMSO} \times N_{carbonate} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{6 \times 2 \times 138}{100 \times 1 \times 78} \times 33\ \mathrm{mg} \times 200 = 1401\ mg$$

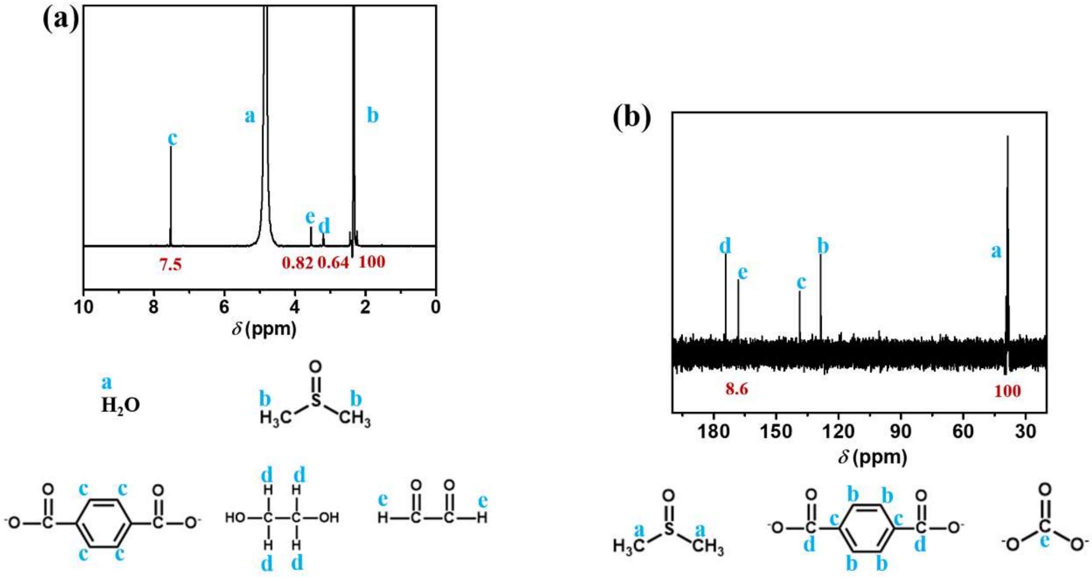


Fig. S7 (a) ^{1}H-NMR and (b) ^{13}C-NMR spectra after PET electroreforming for 15 h.

$$m_{terephthalat} = \frac{I_{terephthala} \times N_{DMSO} \times M_{terephthalate}}{I_{DMSO} \times N_{terephthalat} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{7.5 \times 6 \times 242}{100 \times 4 \times 78} \times 33\ \mathrm{mg} \times 200 = 2303\ mg$$

$$m_{EG} = \frac{I_{EG} \times N_{DMSO} \times M_{EG}}{I_{DMSO} \times N_{EG} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{0.64 \times 6 \times 62}{100 \times 4 \times 78} \times 33\ \mathrm{mg} \times 200 = 50\ mg$$

$$m_{glyoxal} = \frac{I_{glyoxal} \times N_{DMSO} \times M_{glyoxal}}{I_{DMSO} \times N_{glyoxal} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{0.82 \times 6 \times 58}{100 \times 2 \times 78} \times 33\ \mathrm{mg} \times 200 = 121\ mg$$

$$m_{carbonate} = \frac{I_{carbonate} \times N_{DMSO} \times M_{carbonate}}{I_{DMSO} \times N_{carbonate} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{8.6 \times 2 \times 138}{100 \times 1 \times 78} \times 33\ \mathrm{mg} \times 200 = 2008\ mg$$

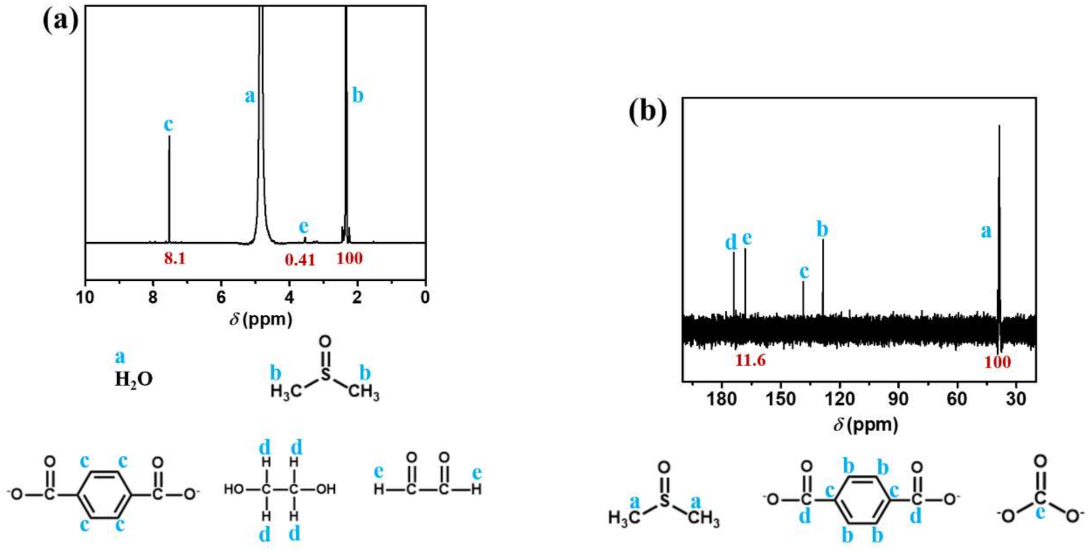


Fig. S8 (a) ^{1}H-NMR and (b) ^{13}C-NMR spectra after PET electroreforming for 20 h.

$$m_{terephthalate} = \frac{I_{terephthalat} \times N_{DMSO} \times M_{terephthalat}}{I_{DMSO} \times N_{terephthalat} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{8.1 \times 6 \times 242}{100 \times 4 \times 78} \times 33\ \mathrm{mg} \times 200 = 2488\ mg$$

$$m_{glyoxal} = \frac{I_{glyoxal} \times N_{DMSO} \times M_{glyoxal}}{I_{DMSO} \times N_{glyoxal} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{0.41 \times 6 \times 58}{100 \times 2 \times 78} \times 33\ \mathrm{mg} \times 200 = 60\ mg$$

$$m_{carbonate} = \frac{I_{carbonate} \times N_{DMSO} \times M_{carbonate}}{I_{DMSO} \times N_{carbonate} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{11.6 \times 2 \times 138}{100 \times 1 \times 78} \times 33\ \mathrm{mg} \times 200 = 2709\ mg$$

$$Selectivity_{carbonate}$$

$$= \frac{m_{carbonate} / M_{carbonate}}{m_{carbonate} / M_{carbonate} + m_{glyoxal} / M_{glyoxal}} \times 100\%$$

$$= \frac{2709/138}{2709/138 + 60/58} \times 100\% = 95\%$$

$EF_{\mathrm{carbonate}} = [5 \times (m_{\mathrm{carbonate}}/M_{\mathrm{carbonate}}) \times F] / Q = [5 \times (2.709/138) \times 96485] / 10183 = 93\%$

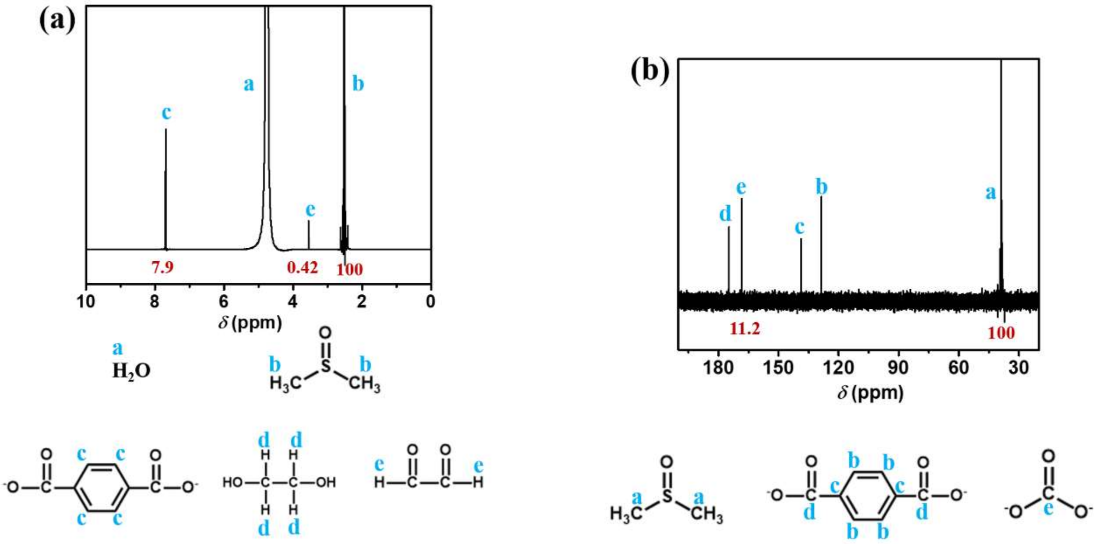


Fig. S9 (a) ^{1}H-NMR and (b) ^{13}C-NMR spectra after PET electroreforming 5 cycles.

$$m_{terephthalat} = \frac{I_{terephthalate} \times N_{DMSO} \times M_{terephthalat}}{I_{DMSO} \times N_{terephthalate} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{7.9 \times 6 \times 242}{100 \times 4 \times 78} \times 33\ \mathrm{mg} \times 200 = 2426\ mg$$

$$m_{glyoxal} = \frac{I_{glyoxal} \times N_{DMSO} \times M_{glyoxal}}{I_{DMSO} \times N_{glyoxal} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{0.42 \times 6 \times 58}{100 \times 2 \times 78} \times 33\ \mathrm{mg} \times 200 = 62\ mg$$

$$m_{carbonate} = \frac{I_{carbonate} \times N_{DMSO} \times M_{carbonate}}{I_{DMSO} \times N_{carbonate} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{11.2 \times 2 \times 138}{100 \times 1 \times 78} \times 33\ \mathrm{mg} \times 200 = 2616\ mg$$

$Selectivity_{carbonate}$

$$= \frac{m_{carbonate} / M_{carbonate}}{m_{carbonate} / M_{carbonate} + m_{glyoxal} / M_{glyoxal}} \times 100\%$$

$$= \frac{2616/138}{2616/138 + 62/58} \times 100\% = 94\%$$

$EF_{\mathrm{carbonate}} = [5 \times (\mathrm{m_{carbonate}/M_{carbonate}}) \times \mathrm{F})]/\ \mathrm{Q} = [5 \times (2.616/138) \times 96485]\ /\ 9850 = 93\%$

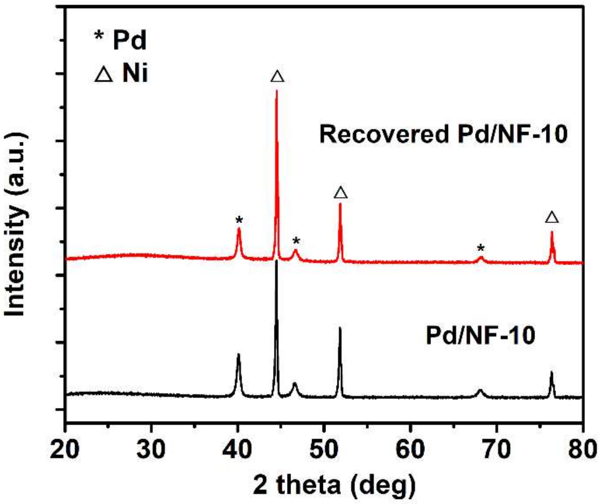


Fig. S10 XRD patterns of Pd/NF-10 and recovered Pd/NF-10 after 5 cycles of PET electroreforming at 0.7 V vs. RHE.

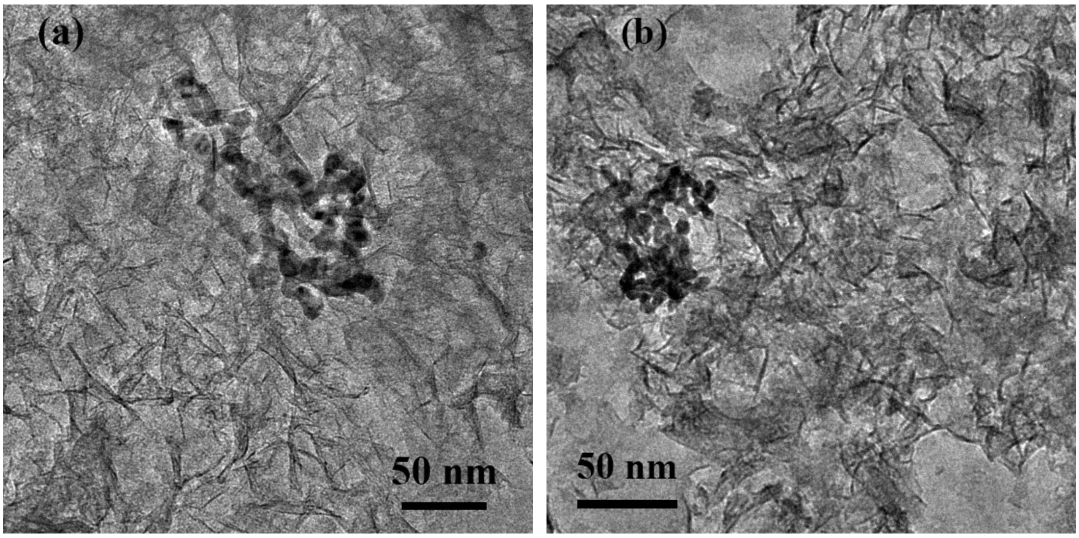


Fig. S11 TEM images of (a) Pd/NF-10 and (b) recovered Pd/NF-10 after 5 cycles of PET electroreforming at 0.7 V vs. RHE.

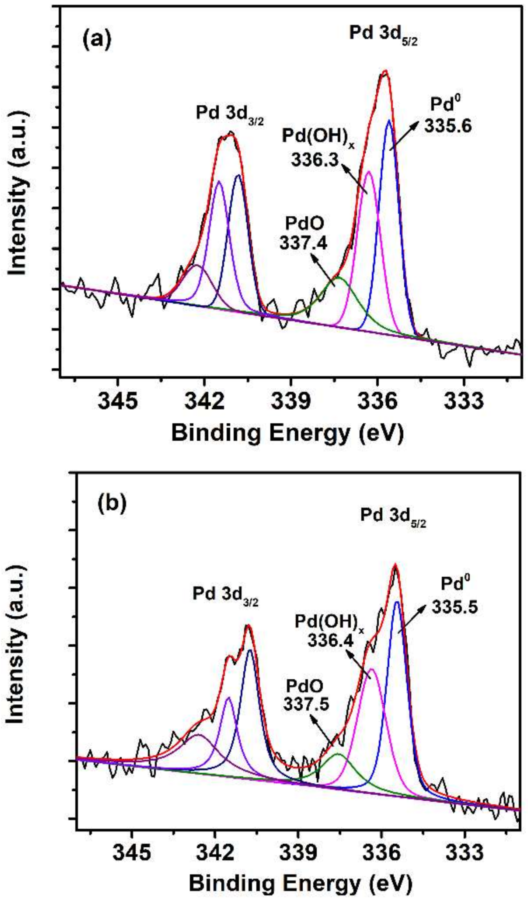


Fig. S12 Pd 3d XPS spectra of (a) Pd/NF-10 and (b) recovered Pd/NF-10 after 5 cycles of PET electroreforming at 0.7 V vs. RHE.

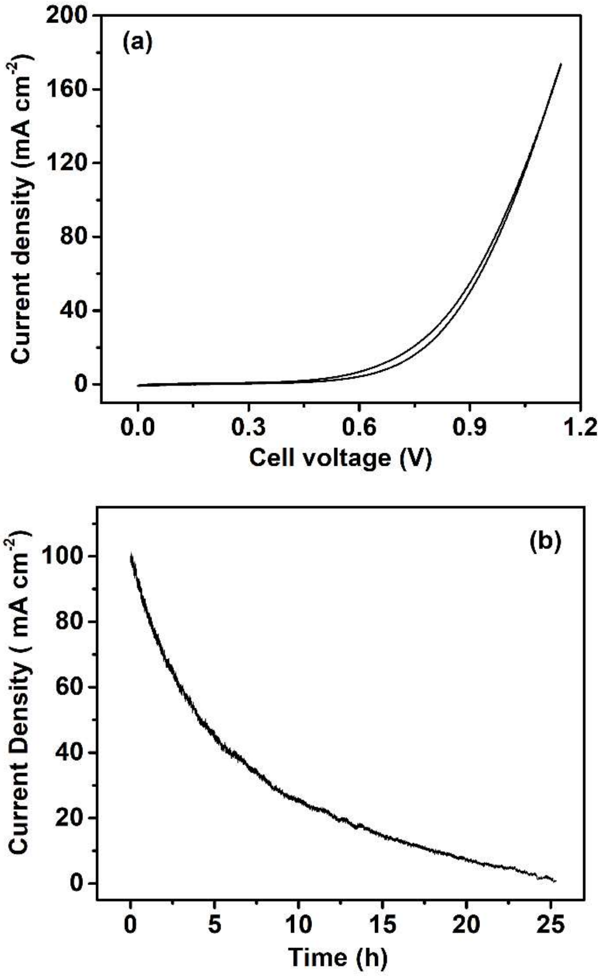


Fig. S13 (a) CV curve of the electroreforming system by using real-world plastic bottles as substrates in a two-electrode system at a scan rate of 10 mV s^{-1}; (b) chronoamperometry curve of the electroreforming system by using real-world PET bottles as substrate in a two-electrode system at a cell voltage of 1.01 V.

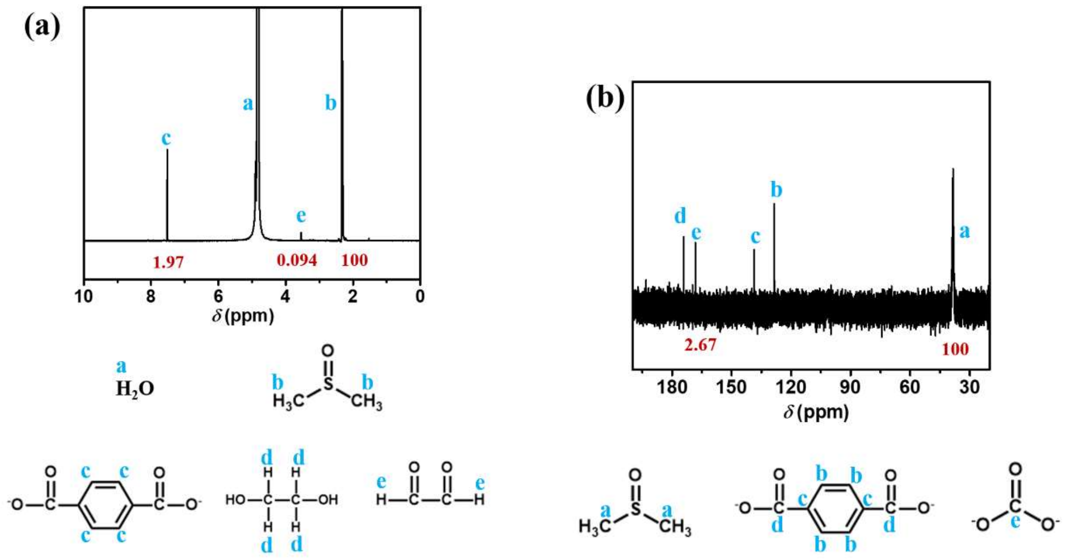


Fig. S14 (a) ^{1}H-NMR and (b) ^{13}C-NMR spectra of real-world plastic bottle after electroreforming.

$$m_{terephthalate} = \frac{I_{terephthalate} \times N_{DMSO} \times M_{terephthalate}}{I_{DMSO} \times N_{terephthalate} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{1.97 \times 6 \times 242}{100 \times 4 \times 78} \times 33\ \mathrm{mg} \times 200 = 605\ mg$$

$$Yield_{terephthalate} = \frac{605\ mg}{630\ mg} \times 100\% = 96\ \%$$

$$m_{carbonate} = \frac{I_{carbonate} \times N_{DMSO} \times M_{carbonate}}{I_{DMSO} \times N_{carbonate} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{2.67 \times 2 \times 138}{100 \times 1 \times 78} \times 33\ \mathrm{mg} \times 200 = 623\ mg$$

$$m_{glyoxal} = \frac{I_{glyoxal} \times N_{DMSO} \times M_{glyoxal}}{I_{DMSO} \times N_{glyoxal} \times M_{DMSO}} \times m_{DMSO} \times n$$

$$= \frac{0.094 \times 6 \times 58}{100 \times 2 \times 78} \times 33\ \mathrm{mg} \times 200 = 13.9\ mg$$

$Selectivity_{carbonate}$

$$= \frac{m_{carbonate} / M_{carbonate}}{m_{carbonate} / M_{carbonate} + m_{glyoxal} / M_{glyoxal}} \times 100\%$$

$$= \frac{623/138}{623/138 + 13.9/58} \times 100\% = 95\%$$

$EF_{\mathrm{carbonate}} = [5 \times (\mathrm{m_{carbonate}/M_{carbonate}}) \times \mathrm{F}] / \mathrm{Q} = [5 \times (0.623/138) \times 96485)]/ 2394 = 91\%$

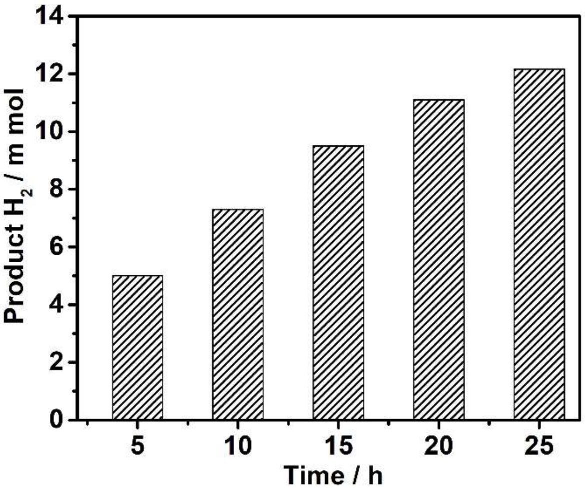


Fig. S15 H_2 evolution during the electroreforming of real-world plastic bottles in a two-electrode system at a cell voltage of 1.01 V.

$EF_{H2} = (2 \times n_{H2} \times F) / Q = (2 \times 0.01216 \times 96485) / 2394 = 98\%$

Herein, we report a electroreforming strategy to upcycle waste PET into high value-added chemicals (carbonate and terephthalate) along with the generation of H_2 using Pd/NF as the anode and Ni foam as the cathode in KOH electrolyte. We subsequently carried out a preliminary techno-economic analysis to evaluate the economic feasibility of the PET electroreforming (Fig. S13). Based on a model reported by Sargent group, it can be estimated that electroreforming per ton of waste PET can get a net profit of ~$560. In this article, PET electroreforming is economically feasible when the faraday efficiency of the electrocatalyst is as high as 91% and the cell voltage is 1.01 V.

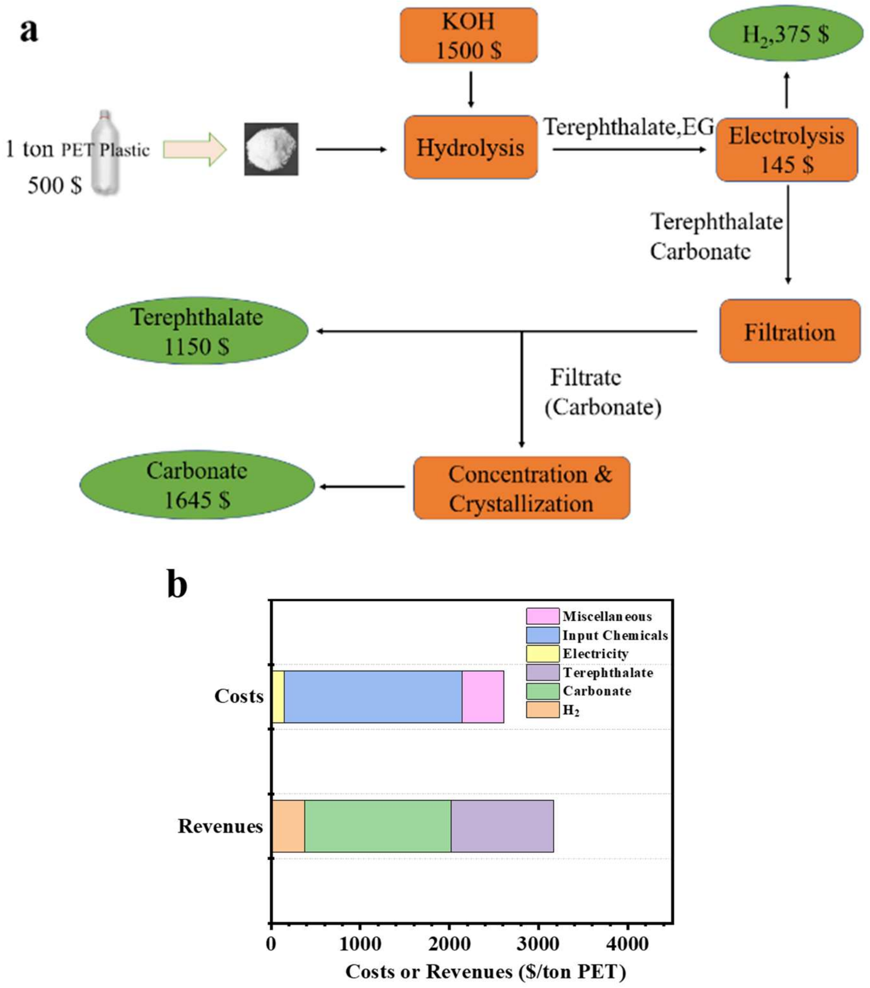


Fig. S16 Electrocatalytic reforming of PET into commercial chemicals and H_2 fuel. (a) Schematic illustration of the electroreforming process and the final products are terephthalate, carbonate, and H_2. (b) Techno-economic analysis of this process. Assuming 100% of terephthalate and 100% of carbonate are recycled.

The calculation process:

1. Electricity costs:

The total charge required for electrolysis per ton of PET can be calculated as follows:

$$Q = \frac{\mathrm{m} \times \mathrm{F} \times \mathrm{N}}{\mathrm{M} \times \mathrm{FE}}$$

Where Q is the total charge, m is the mass of ethylene glycol, F is the Faraday's constant and N takes the value 2, M is the molar mass of ethylene glycol, FE is the faradaic efficiency of carbonate from PET electro-reforming.

The current with a capacity factor of 0.8 can be calculated as follows:

$$I = \frac{\mathrm{Q}}{\mathrm{T} \times \mathrm{CF}}$$

Where I is the current, T is the time in a day, CF is the capacity factor.

The power required to maintain electrolysis process can be calculated as follows, assuming that the cell potential is 1.01 V:

$$P = \frac{\mathrm{U} \times \mathrm{I}}{1000} (kw)$$

The electricity cost for electrolysis can be calculated as follows:

$$\text{Electrolyzer electricity cost} = \mathrm{P} \times \mathrm{T} \times \mathrm{CF} \times \text{Cost per KWh}$$

It is assumed that the electricity cost required for the hydrolysis process is equivalent to that of the electrolysis process:

Hydrolysis electricity cost = Electrolyzer electricity cost

Thus, the total electricity cost can be calculated as:

Total electricity cost

= Hydrolysis electricity + Electrolyzer electricity cost

2. Input chemicals costs: 1 ton PET, 1.75 ton KOH and 375 kg water.

Input chemicals = Price of PET (500 $/ton) × Mass of PET + Price of KOH (850 $/ton) × Mass of KOH + Price of water (0.22 $/ton) × Mass of water.

3. Miscellaneous costs: In the electro-reforming PET process, miscellaneous costs including capital costs, maintenance costs, installation costs, and operating costs are 465 $ / ton PET according to the reference.[2]

Finally, the total cost of the electro-reforming PET process can be calculated:

Total costs = Input chemicals + Electricity cost + Miscellaneous costs

Electro-reforming per ton of PET can obtain 1.26 ton potassium terephthalate, 1.44 ton potassium carbonate, and 0.052 ton H_2.

So the profit of the product can be calculated as:

Product value = Price of potassium terephthalate (915 \$/ton) × Mass of obtained potassium terephthalate + Price of potassium carbonate (1145 \$/ton) × Mass of obtained potassium carbonate + Price of H_2 (7210 \$/ton) × Mass of obtained H_2.

Therefore, the total income of electrolysis per ton of PET can be calculated as follows:

Total profit per ton of PET = Product value per ton of PET – Total costs per ton of PET.

Reference

1. H. Xu, B. Yan, K. Zhang, J. Wang, S. Li, C. Wang, Y. Du, and P. Yang, *Electrochim. Acta.*, 2018, **261**, 521-529.
2. H. Zhou, Y. Ren, Z. H. Li, M. Xu, Y. Wang, R. X. Ge, X. G. Kong, L. R. Zheng and H. H. Duan *Nat. Commun.*, 2021, **12**, 4679.