Supporting Information

Supramolecular electrocatalysis on high efficient oxygen evolution reaction with cucurbit[6]uril

Xin Dai[1], Xian-Yi Jin[1], Qingmei Ge[1], Jie Zhao[1], Mao Liu[1], Hang Cong[1,*], Zhu Tao[2] and Nan Jiang[1,*]

[1]Enterprise Technology Center of Guizhou Province, Guizhou University, Guiyang 550025, China.

E-mail: hcong@gzu.edu.cn for H. Cong, nan.jiang@unlv.edu for N. Jiang

[2]Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang 550025, China.
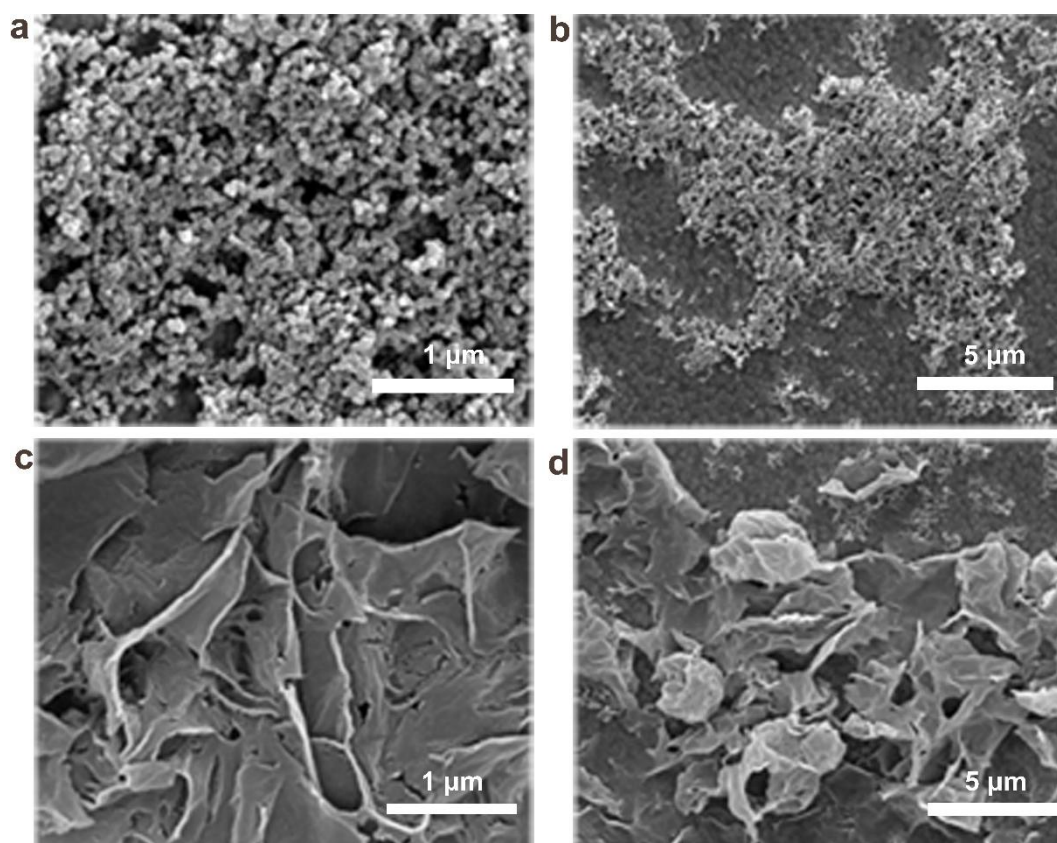
Figure S1. SEM images of (a) and (b) PPy; (c) and (d) PPy@rGO
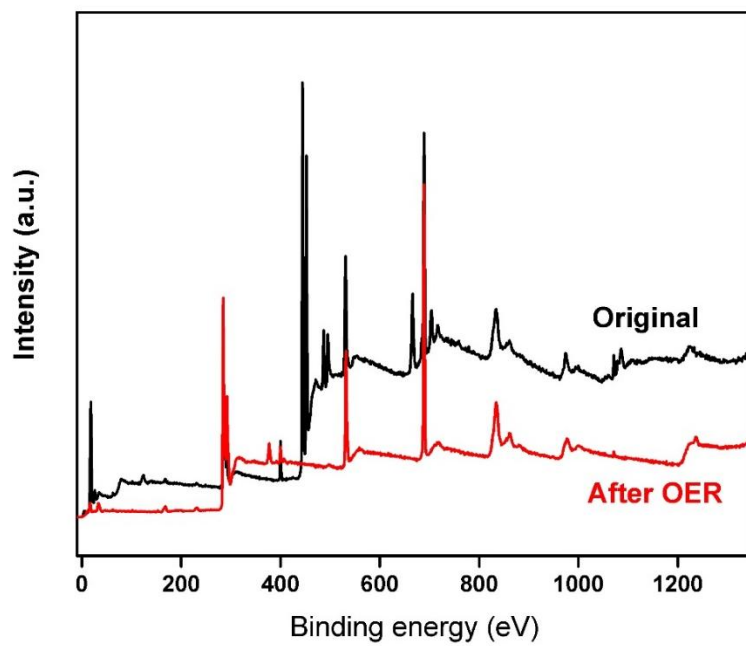
Figure S2. XPS survey spectra of PPy@rGO@Q[6] for the OER before (black lines) and after (red lines) stability test.
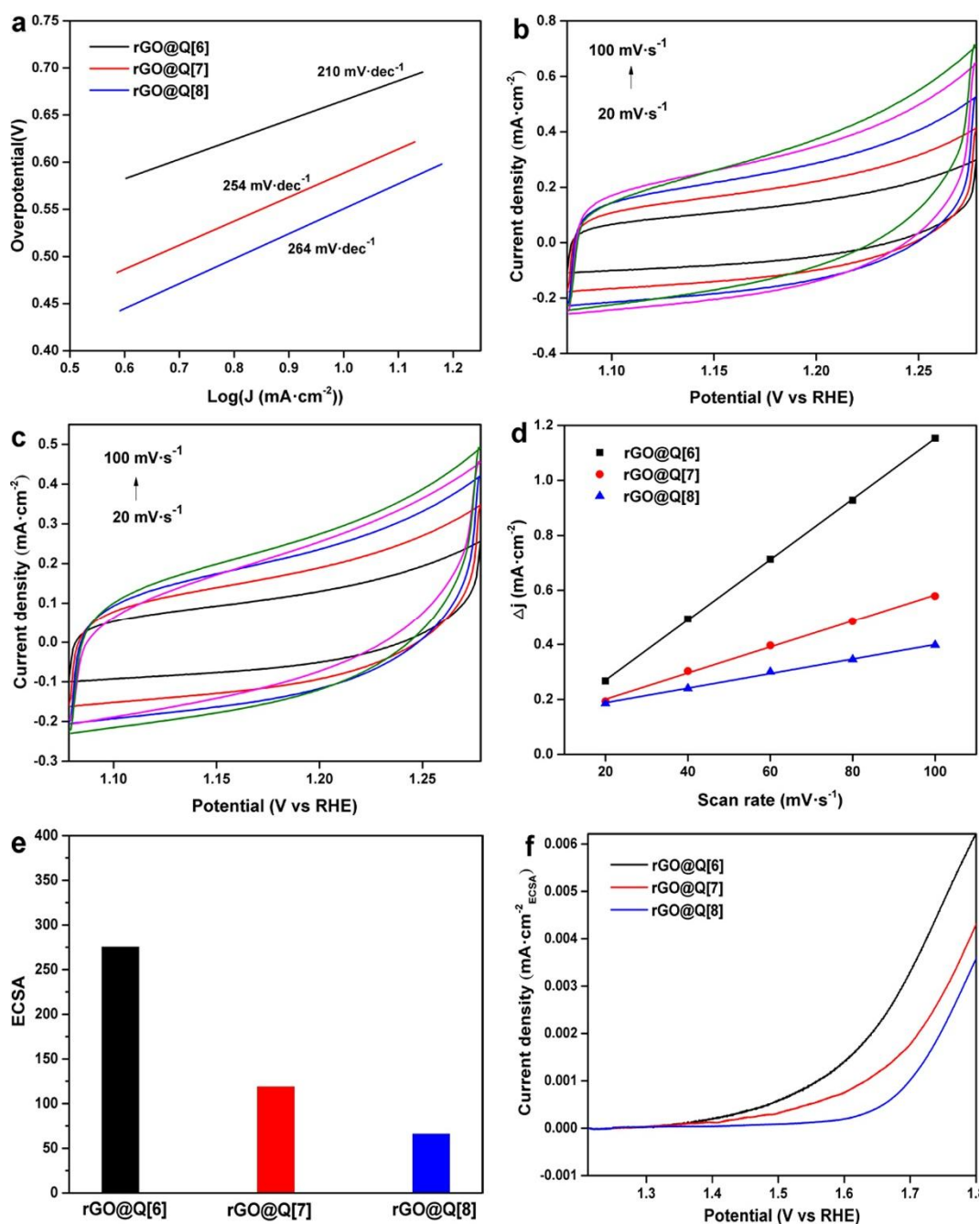
Figure S3. (a) Corresponding Tafel slopes of the stepwise-coating catalysts for the OER in 1.0 M KOH; (b) the CVs at different scan rates (20-100 mV·s⁻¹) for rGO@Q[7]; (c) the CVs at different scan rates (20-100 mV·s⁻¹) for rGO@Q[8]; (d) the trend of C_{dl} values for the catalysts in 1.0 M KOH; (e) corresponding ECSA of the stepwise-coating catalysts; (f) LSV curves of different samples normalized to (e) ECSA.

According to the LSV curves (Figure 3a), the Tafel slope of 210 mV·dec⁻¹ for rGO@Q[6] was determined to be much smaller than the values of rGO@Q[7] (254 mV·dec⁻¹) and rGO@Q[8] (258 mV·dec⁻¹), suggesting more favorable and fast catalytic OER kinetics for rGO@Q[6] (Figure S3a). In addition, electrochemical active surface areas (ECSA) were also estimated by calculating the double-layer capacitances (C_{dl}) via cyclic voltammograms (CVs) at different scan rates from 20

mV·s^{-1} to 100 mV·s^{-1}(Figure S3b, S3c, S3d and S3e). The higher values of C_{dl} and ECSA for rGO@Q[6] (11.03 mF·cm^{-2}, 275.75 cm^{-2}) than rGO@Q[7] (4.77 mF·cm^{-2}, 119.25 cm^{-2}) and rGO@Q[8] (2.65 mF·cm^{-2}, 66.25 cm^{-2}) also indicated that rGO@Q[6] had a higher electrocatalytic activity. To consider the intrinsic activities of the different samples, the LSV curves were normalized to ECSA, respectively (Figure S3f, ESI). The results still displayed the best OER activity of rGO@Q[6], confirming the highest intrinsic activity. Furthermore, Figure S4 (ESI) described the Nyquist plots of the samples, the smaller semicircle diameter was found in the case of rGO@Q[6], which indicated that the R_{ct} value of rGO@Q[6] (3.92 Ω) was much lower than those of rGO@Q[7] (4.52 Ω) and rGO@Q[8] (5.13 Ω). Hence, compared with the rGO@Q[7] and rGO@Q[8] , the rGO@Q[6] produced lower charge transfer resistance and better electronic transport capability.
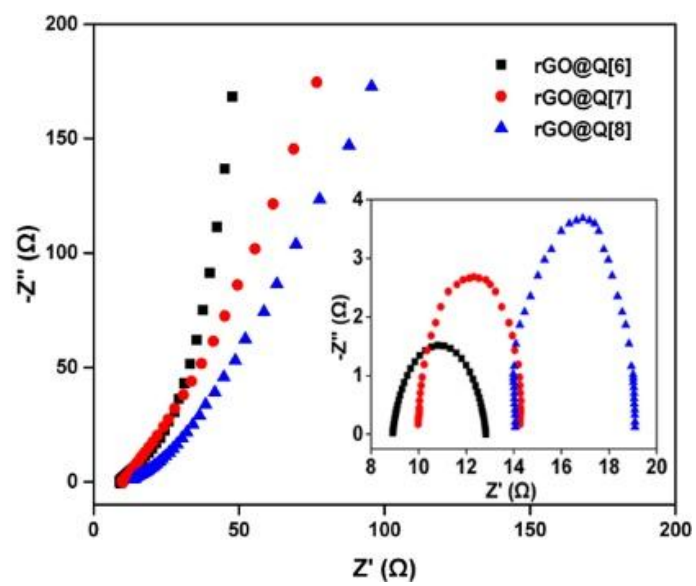
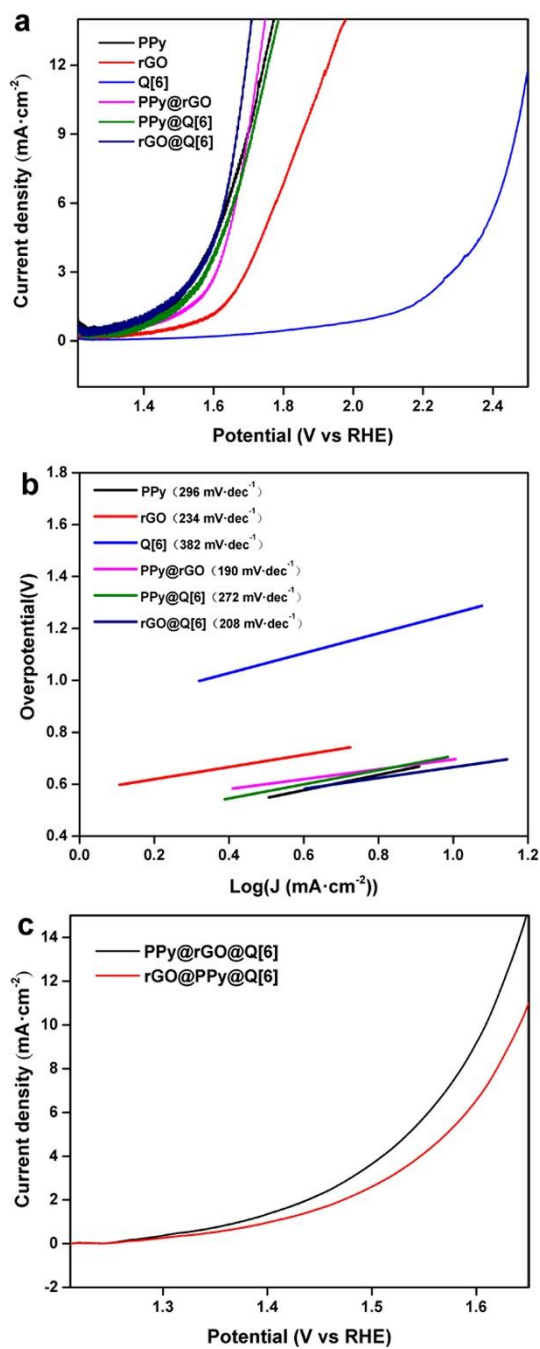Figure S4. Nyquist plots of the catalysts.

Figure S5. (a) LSV curves of the catalysts with layer-by-layer coating for the OER in 1.0 M KOH; (b) corresponding Tafel slopes of the stepwise-coating catalysts; (c) LSV curves of PPy@rGO@Q[6] and rGO@Q[6]@PPy in 1.0 M KOH.
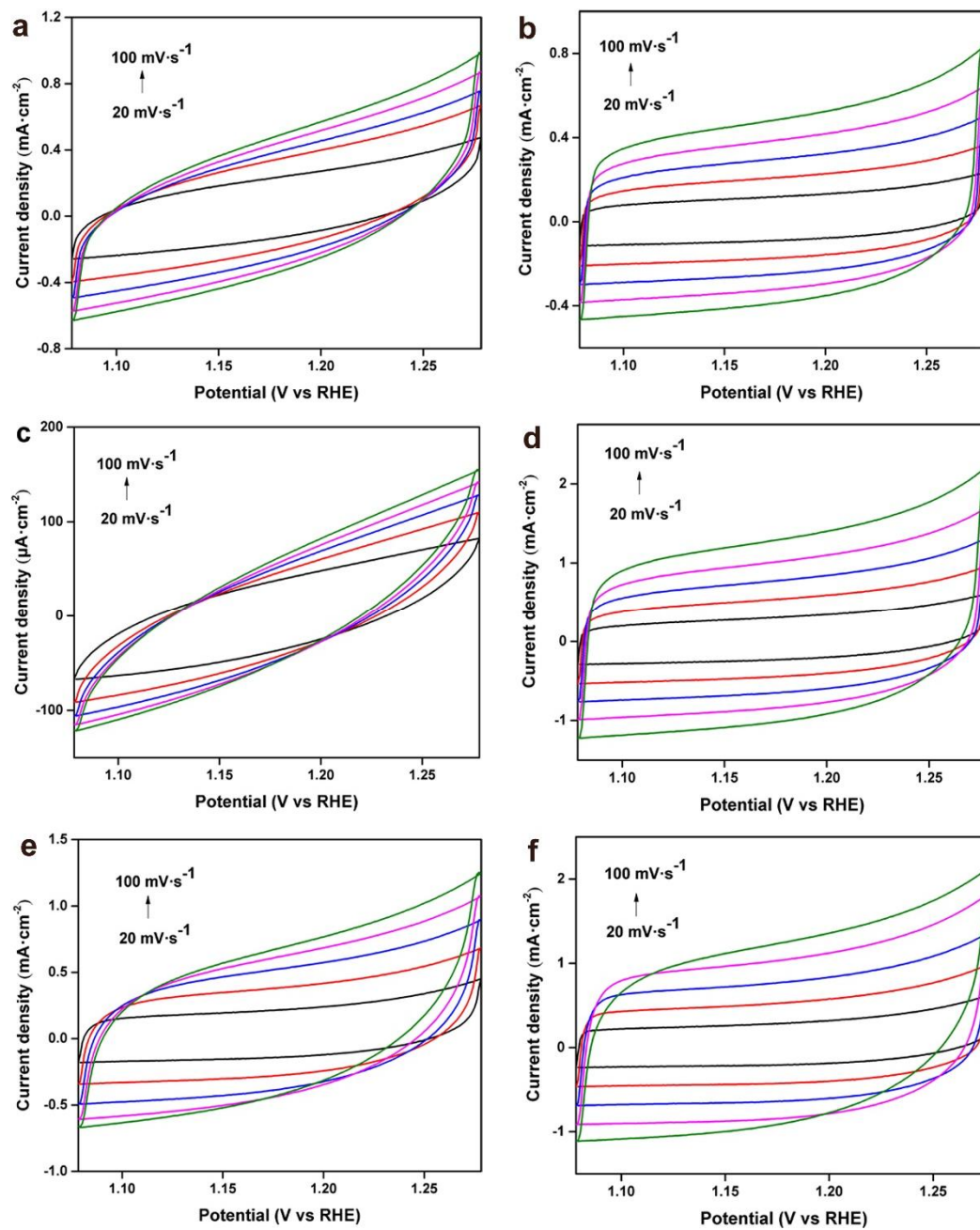
Figure S6. The CVs at different scan rates (20-100 mV·s−1) for (a) PPy; (b) rGO; (c) Q[6]; (d) PPy@rGO; (e) PPy@Q[6]; (f) rGO@Q[6]
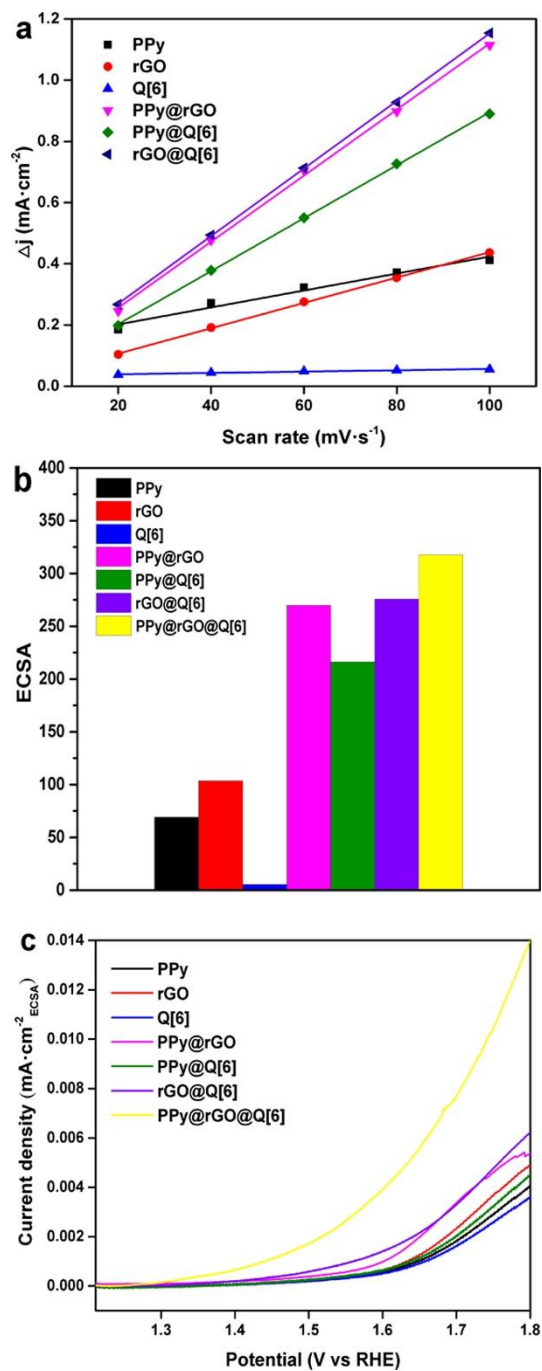
Figure S7. (a) The trend of C_{dl} values for the catalysts in 1.0 M KOH; (b) corresponding ECSA of the stepwise-coating catalysts; (c) LSV curves of different samples normalized to (b) ECSA.
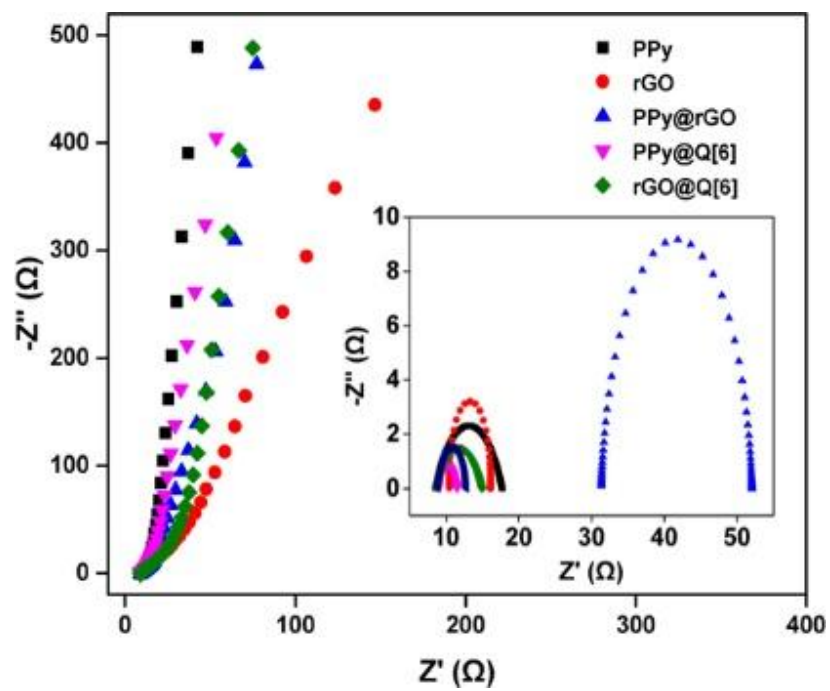
Figure S8. Nyquist plots of the catalysts measured at 377 mV

Table S1. The R_s and R_{ct} of PPy@rGO@Q[6] extracted from fitting electrochemical impedance spectra measured at different potential to an equivalent circuit

Potential / mV (vs. Ag/AgCl)	R_s / Ω	R_{ct} / Ω
357 mV	8.348	2.34
367 mV	8.564	1.49
377 mV	8.544	1.45
387 mV	8.759	1.16
397 mV	8.577	1.07
407 mV	8.956	1.06

Table S2. The R_s and R_{ct} of the different catalysts extracted from fitting electrochemical impedance spectra measured at 377 mV

Catalysts	R_s / Ω	R_{ct} / Ω
PPy	8.56	9.16
rGO	10.47	5.62
Q[6]	31.32	20.73
PPy@rGO	8.96	2.56
PPy @Q[6]	8.57	6.39
rGO@Q[6]	8.91	3.92
PPy@rGO@Q[6]	8.76	1.16

Table S3. Faradaic efficiency (FE) of the produced oxygen amount during the water splitting process

Times/s	V/ mL	FE / %
1200	0.65	93.32
2400	1.35	96.91
3600	2	95.72
4800	2.7	96.92
6000	6.4	97.63