Supporting Information

Oxygen Evolution Reaction at Carbon Edge Sites: Investigation of Activity Evolution and Structure–Function Relationships with Polycyclic Aromatic Hydrocarbons

Yangming Lin, Qing Lu, Feihong Song, Linhui Yu, Anna K. Mechler, Robert Schlögl, and Saskia Heumann*

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Materials

Phenanthrene (PT, $\geq 99.5\%$), anthracene (AT, $\geq 99\%$) and naphthacene (NT, 99.99\%) were obtained from Aldrich. All chemicals were used as received without further purification. Dibenzo[b,def]chrysene (DC, $\geq 98\%$) was purchased from TCI. Cyclohexane was purchased from Merck Co. (Germany). Purified ultra-dispersed nanodiamond (UDD) was bought from Beijing Grish Hitech Co. (China). The surface area of OLC is about 460 m$^2$/g. HHT was bought from Pyrograf Products, Inc. The surface area of HHT is about 34 m$^2$/g. All the two carbon materials were purified in concentrated HCl at room temperature for 20 h to remove the metal impurities before use.

Synthesis of onion-like carbon (OLC)

OLC with graphite-like shell structures was prepared by annealing purified nanodiamond at 1500 °C for 30 min in argon atmosphere. The yield of OLC was about 75%. The surface area of OLC is about 460 m$^2$/g.

Synthesis of supported HHT and onion-like carbon (OLC)

In a typical procedure, 100 mg HHT and 20 mg of model catalysts, such as phenanthrene (PT), anthracene (AT), were dissolved in 70 mL of cyclohexane to form a mixture which was then sonicated for 30 min under the room temperature. The obtained mixture was then transferred into a Teflon-lined stainless steel autoclave with a capacity of 200 mL and 400 rpm rotation rate and maintained at about 100 °C for 24 h. The final products were filtered and washed with a large amount of ethanol to clear the excess of model catalysts and cyclohexane and then dried it at 70 °C for 12 hours. The as-prepared supported HHT were labeled as PT+HHT, AT+HHT, NT+HHT and DC+HHT, respectively. Pure HHT was treated by the same process without the introduction of model catalysts and acted as a reference materials (labeled by T-HHT). The T-OLC and supported OLC samples were prepared by using the same procedure.
Materials Characterization

High-resolution transmission electron microscopy (HRTEM) images were achieved on a FEI Tecnai G2 F20 microscope. Thermogravimetric (TG) analysis was performed on a NETZSCH STA449 F3 thermal analyzer. The atmosphere was argon, and the heating rate was 10 °C/min from 40 °C to 1000 °C. Electrochemical measurements were performed using an potentiostat/galvanostat (BioLogic VSP, France) with a conventional three-electrode electrochemical cell. A platinized Pt wire as a counter electrode and a reversible hydrogen electrode (RHE, HydroFlex, Gaskatel GmbH) as a reference electrode were used. The glassy carbon electrode (GCE, 5 mm diameter, 0.196 cm²) with rotating disk electrode (RDE) as a working electrode was polished by 0.1 µm and 0.05 µm alumina powder and rinsed with deionized water, followed by sonication in ethanol and deionized water. The modified samples were transferred onto the GCE according to the following procedures: (1) 5 mg catalysts were added into the mixture solution of 960 ul H₂O, 4 mL isopropanol and 40 µL nafion, and then ultrasonicated for 15 min. (2) 10 µL of as-made mixture solution was dropped on the GCE surface and dried at 60 °C for few minutes in air. The final loading of catalyst on electrode is about 0.051 mg/cm². Cyclic voltammograms (CVs) were obtained by scanning between 0 V to 1.0 V at a scan rate of 100 mV/s in argon-saturated solution. OER polarization curves were obtained by linear sweep voltammetry scanning from 1.0 V to 1.8 V~1.9V at a scan rate of 5 mV/s in argon-saturated 0.1 M KOH with RDE (rotation rate of 1600 rpm). Prior to the impedance measurements, the electrodes were held at a constant desired potential for 10 min to ensure a stable current. And then measurements were performed by applying an AC voltage with 5 mV amplitude in a frequency range from 100 kHz to 100 mHz. All the experiments were carried out at room temperature. The calculation of electrochemically active surface area (ECSA) is based on the measured double layer capacitance of the pure HHT and supported HHT on glassy carbon RDE in 0.1M KOH according to a previous published report. Briefly, a potential range where no apparent Faradaic process happened was determined firstly using the static CV. This range is typically a 0.1 V potential window centered at the open-circuit potential (OCP) of the system. All measured current in this non-Faradaic potential region is assumed to be due to double-layer charging.[1] The charging current, iₙ, is then measured from CVs at different scan rates. The working
electrode was held at each potential vertex for 10 s before beginning the next sweep. The relation between $i_c$, the scan rate ($\nu$) and the double layer capacitance ($C_{dl}$) was given in equation 1.

$$C_{dl} = \frac{i_c}{\nu}$$  \hspace{1cm} (1)

Therefore, the value of $C_{dl}$ can be obtained from the slope of $i_c$ as a function of $\nu$.

For the calculation of ECSA, a specific capacitance ($C_s$) value $C_s \approx 0.019$ mF cm$^{-2}$ (estimated value) in 0.1 M NaOH is adopted from previous reports.[2] The relative equation is:

$$\text{ECSA} = \frac{C_{dl}C_s}{\nu}$$  \hspace{1cm} (2)

Reference

[1] C. C. L. McCrory, S. Jung, J. C. Peters, T. F. Jaramillo, Benchmarking heterogeneous electrocatalysts for the oxygen evolution reaction. *J. Am. Chem. Soc.*, 2013, 135, 16977-16987.

[2] W. A. Badawy, A. G. Gad-Allah, H. A. Abd El-Rahman, M. M. Abouromia, Kinetics of the passivation of molybdenum in acids and alkali solutions as inferred from impedance and potential measurements. *Surf. Coat. Tech.*, 1986, 27, 187-196.

Mass spectra measurement was performed on an OmniStar™ GSD 320 mass spectrometer purchased from PFEIFFER VACUUM Ltd. The detector type is C-SEM/Faraday. The carry gas was Ar with a flow rate of 1 mL/s. The O$_2$ was collected after 12 h at a constant potential of 1.6 V vs RHE using a home-made cell with glass carbon pellet (the diameter is 1cm) as working electrode. The loading of AT+HHT catalyst on electrode are 0.5 mg/cm$^2$.

Calculation Method

1. TOF values
The theoretical values of TOF were calculated by assuming that every edge groups is involved in the catalysis.

\[
\text{TOF} = \frac{(j \times S) \times \text{FE}}{(4 \times F \times n)}
\]

Where \( j \) is the measured current density at \( \eta = 0.370 \text{ V} \) and \( S \) is the surface area of glass carbon disk (0.196 cm\(^2\)). \( F \) represents Faraday constant (96485.3 C mol\(^{-1}\)), and the number 4 means 4 electrons/mol of \( \text{O}_2 \). \( n \) is the moles of the pure model catalysts that are deposited onto the glass carbon disk. Prior to the calculation of TOF, the relevance mass fraction of pure model catalysts is obtained from TG. By using this equation, the TOF values can be obtained based on per model molecule. Moreover, the different theoretical TOF values based on the per carbon atom and outer carbon atom of the model molecules are also calculated. In the present work, to gain the more accurate results, the faradic efficiencies (FE) of catalysts for oxygen evolution are included in the calculation of the theoretical TOF.

The Tafel slope was calculated according to Tafel equation as follows:

\[
\eta = b \cdot \log\left(\frac{j}{j_0}\right)
\]

where \( \eta \) denotes the overpotential, \( b \) denotes the Tafel slope, \( j \) denotes the current density, and \( j_0 \) denotes the exchange current density.

2. Faradaic efficiency (FE)

In order to study the reaction mechanism for OER, rotating ring-disk electrode (RRDE) voltammograms were carried out based on a Pt ring electrode and a glassy carbon disk electrode. The as-obtained AT-supported HHT catalyst was drop-cast onto the RRDE using above method. To detect the content of the formed peroxide intermediates, the ring potential was fixed constantly at 1.465 V vs. RHE in Ar-saturated 0.1 M KOH solution and recorded the data under a rotation rate of 1600 rpm at a scan rate of 5 mV/s\(^{-1}\). The \( \text{HO}_2^- \) intermediate production percentage (\( \% \text{ HO}_2^- \)) were determined as follows:

\[
\% \text{HO}_2^- = \frac{200I_r}{(I_dN + I_r)}
\]

where \( I_d \) is the disk current, \( I_r \) is the ring current and \( N \) is the current collection efficiency (26%). In the present RRDE system, the outer diameter of disk is 5.0 mm; the outer diameter of ring is 7.50 mm.
and the inner diameter of ring is 6.5 mm. The RRDE photograph is displayed in Figure S1.

**Figure S1.** The photograph of RRDE

The Faradaic efficiency (FE) of the system was measured to ensure that the oxidation current derived from oxygen evolution rather than other side reactions. Here, the ring potential was held constantly at 0.465 V vs. RHE to reduce the O$_2$ formed from the catalyst on the disk electrode in Ar-saturated 0.1 M KOH solution. The FE determined as follows $^{[1,3]}$:

$$\text{FE} = \frac{j_r}{j_d N}$$

Where $j_r$ is the ring current density, $j_d$ is the current density of the disk electrode and $N$ is the current collection efficiency (26%). Here, the selected ring potential (0.465 V) can not trigger CO$_2$ reduction.$^{[4]}$

[3] X. Lu, W.-L. Yim, B. H. Suryanto, C. Zhao, Electrocatalytic oxygen evolution at surface-oxidized multiwall carbon nanotubes, *J. Am. Chem. Soc.*, 2015, 137, 2901-2907.

[4] T. Liu, S. Ali, Z. Lian, B. Li, D. S. Su, CO$_2$ electoreduction reaction on heteroatom-doped carbon cathode materials, *J. Mater. Chem. A*, 2017, 5, 21596-21603.

3. KIE values

KIE values are defined by the ratio of the isotopic rate constants ($k_0^H/k_0^D = k_H/k_D$). $k_H/k_D$ can be calculated by the exchange current densities on a catalyst in H$_2$O ($j_0^H$) and D$_2$O water ($j_0^D$), that is,

$$\text{KIE} = \frac{k_H}{k_D} = \frac{j_0^H C_0^D}{j_0^D C_0^H}$$

where $C_0$ is the O$_2$ concentration in H$_2$O or D$_2$O. The value of $C_0^D/C_0^H$ is defined to be 1.101 at 298 K. Exchange current densities ($j_0$) can be calculated by
\[ j = j_0 \exp(n \alpha \eta / RT) \]

where \( n, \alpha, F, R, \) and \( T \) denote the number of electrons involved in the electrode reaction number (it is 4 in the OER process), transfer coefficients, Faraday constant, gas constant (8.314 J K\(^{-1}\) mol\(^{-1}\)), and reaction temperature (298 K), respectively. The \( \alpha \) can be calculated from the Tafel slope \( b \) (V dec\(^{-1}\)), that is

\[ b = \frac{2.303RT}{n \alpha F} \]
\[ \alpha = \frac{0.0592}{4b} \]

Here, Tafel slope of NT+HHT is 0.066 V dec\(^{-1}\). The \( \alpha \) value can be calculated to be 0.224.
Scheme S1. The synthetic process of PAHs-supported HHT and onion-like carbon (OLC).
Figure S2. HRTEM image and Raman spectrum of HHT. The value of $I_D/I_G$ is calculated from peak area. The surface area of HHT is about 34 m$^2$/g. The conductivity of HHT is about 15 S/cm.

[5] G. Wen, S. Wu, B. Li, C. Dai, D. S. Su, Active Sites and Mechanisms for Direct Oxidation of Benzene to Phenol over Carbon Catalysts, Angew. Chem. Int. Ed., 2015, 54, 4105-4109.

[6] D. V. P. Sanchez 1, D. Jacobs, K. Gregory, J. Huang, Y. Hu, R. Vidic, M. Yun, Changes in Carbon Electrode Morphology Affect Microbial Fuel Cell Performance with Shewanella oneidensis MR-1, Energies, 2015, 8, 1817-1829.
Figure S3. HRTEM image and Raman spectrum of onion-like carbon (OLC). The value of I_D/I_G is calculated from peak area. The surface area of OLC is about 460 m$^2$/g.\textsuperscript{[7]} The conductivity of OLC is about 0.8 S/cm.\textsuperscript{[8]}

\textsuperscript{[7]} Y. Lin, B. Li, Z. Feng, Y. A. Kim, M. Endo, D. S. Su, Efficient Metal-Free Catalytic Reaction Pathway for Selective Oxidation of Substituted Phenols,\textit{ACS Catal.}, \textbf{2015}, 5, 5921-5926.

\textsuperscript{[8]} Y. Lin, Z. Feng, L. Yu, Q. Gu, S. Wu, D. S. Su, Insights into the surface chemistry and electronic properties of sp$^3$ and sp3-hybridized nanocarbon materials for catalysis,\textit{Chem. Commun.}, \textbf{2017}, 53, 4834-4837.
Figure S4. IR spectra recorded in attenuated total reflectance (ATR) mode of pure AT powder (red), pure solvent (cyclohexane, black), dissolved AT (cyclohexane as solvent, blue) at 100 °C for 24 h and exfoliated AT (turquoise). Here, the exfoliated AT was obtained by removing the AT molecules from as-prepared AT+HHT sample with sonication method for 8 h in cyclohexane.

As shown in Figure S4, the main characteristic peaks of pure AT powder located at 720 and 881 cm\(^{-1}\) are corresponded to vibration of aromatic rings. When pure AT powder is dispersed in cyclohexane (AT+solvent), the similar characteristic peaks on the obtained solution are observed in the solution. It is clearly seen that the exfoliated AT molecules from the as-prepared AT+HHT sample using sonication method also show the main characteristic peaks of aromatic rings. The slight shift of peaks can be attributed to the change of π-π interaction between AT molecules in solvent. The measurements confirm that the aromatic structure of AT is not destroyed during the preparation process and that the structure is also present while the organic molecule is adsorbed on the support surface.
Figure S5. IR spectra recorded in ATR mode of pure PT powder (red), pure solvent (cyclohexane, black), dissolved PT (cyclohexane as solvent, blue) at 100 °C for 24 h and exfoliated PT (turquoise). Here, the exfoliated PT was obtained by removing the PT molecules from as-prepared PT+HHT sample with sonication method for 8 h in cyclohexane.

As shown in Figure S5, the main characteristic peaks of pure PT powder located at 729 and 813 cm⁻¹ are ascribed to vibration of aromatic rings. When pure PT powder is dispersed in cyclohexane, the similar characteristic peaks on the obtained solution are observed. It is clearly seen that the exfoliated PT molecules from as-prepared PT+HHT sample using sonication method also show the main characteristic peaks of aromatic rings. The slight shift of peaks can be attributed to the change of π-π interaction between PT molecules in solvent. The measurements confirm that the aromatic structure of PT is not destroyed during the preparation process and that the structure is also present while the organic molecule is adsorbed on the support surface.
**Figure S6.** Theoretical TOF values of PT- and AT-supported HHT catalysts at 1.6 V vs RHE based on per carbon atom and per outer carbon atom. Here, we assume that there are six outer zigzag-type/armchair-type carbon atoms in individual AT or PT molecule.

**Figure S7.** Tafel slopes of various catalysts.
Figure S8. Nyquist plots of the pure AT, T-HHT and AT-supported HHT catalysts recorded at 1.6 V. Smaller semicircle diameter imply a better charge transfer at the electrode/electrolyte interface.

Figure S9. Detection of H\textsubscript{2}O\textsubscript{2} and O\textsubscript{2} evolution from (a) AT- and (b) PT- supported HHT applying rotating ring disk electrode (RRDE) measurements. The Pt ring was biased at 1.465 V versus RHE to collect H\textsubscript{2}O\textsubscript{2} and fixed at 0.465 V versus RHE to collect O\textsubscript{2} in Ar-saturated 0.1 M KOH. The current collection efficiency is 26\%.
Figure S10. Electrochemical CV spectra of T-HHT, pure AT and AT-supported HHT at 1.6V after 2 h.
**Figure S11.** The net contents of NT and DC molecules on supported HHT catalyst with TG measurement.
Figure S12. IR spectra recorded in ATR mode of pure NT powder (red), pure solvent (cyclohexane, blue), dissolved NT (cyclohexane as solvent, black) at 100 °C for 24 h and exfoliated NT (turquoise). Here, the exfoliated NT was obtained by removing the NT molecules from as-prepared NT+HHT sample with sonication method for 8 h in cyclohexane.

As shown in Figure S12, the main characteristic peaks of pure NT powder located at 738 and 903 cm⁻¹ are assigned to vibration of aromatic rings. When pure NT powder is dispersed in cyclohexane, the similar characteristic peaks on the obtained solution are observed. It is clearly seen that the exfoliated NT molecules from as-prepared NT+HHT sample using sonication method also show the main characteristic peaks of aromatic rings. The slight shift of peaks can be ascribed to the change of π-π interaction between NT molecules in solvent. The measurements confirm that the aromatic structure of NT is not destroyed during the preparation process and that the structure is also present while the organic molecule is adsorbed on the support surface.
Figure S13. IR spectra recorded in ATR mode of pure DC powder (red), pure solvent (cyclohexane, black), dissolved DC (cyclohexane as solvent, blue) at 100 °C for 24 h and exfoliated DC (turquoise). Here, the exfoliated DC was obtained by removing the DC molecules from as-prepared DC+HHT sample with sonication method for 8 h in cyclohexane.

As shown in Figure S13, the main characteristic peaks of pure DC powder located at 738, 756 and 873 cm⁻¹ are attributed to vibration of aromatic rings. When pure DC powder is dispersed in cyclohexane, the similar characteristic peaks on the obtained solution are observed. It is clearly seen that the exfoliated DC molecules from as-prepared DC+HHT sample using sonication method also show the main characteristic peaks of aromatic rings. The slight shift of peaks can be assigned to the change of π-π interaction between DC molecules in solvent. All the results indicate that the aromatic structure of DC is not destroyed during the preparation process. The measurements confirm that the aromatic structure of DC is not destroyed during the preparation process and that the structure is also present while the organic molecule is adsorbed on the support surface.
Figure S14. Tafel slopes of various PAHs-supported catalysts.
Figure S15. Detection of H$_2$O$_2$ and O$_2$ evolution from (a) NT- and (b) DC- supported HHT applying RRDE measurements. The Pt ring was biased at 1.465 V versus RHE to collect H$_2$O$_2$ and fixed at 0.465 V versus RHE to collect O$_2$ in Ar-saturated 0.1 M KOH. The current collection efficiency is 26%. 
Table S1. Comparison of the electrocatalytic OER activity of the highly active transition-metal and carbon-supported catalysts. Here, $\eta$ is overpotential.

| Reported Catalysts       | $\eta$ (mV) | Electrolyte | TOF@$\eta$ | Literature                  |
|--------------------------|-------------|-------------|------------|-----------------------------|
| NiFe LDHs                | 300         | 1M KOH      | 0.05 s$^{-1}$ | Nat. Commun. 2014, 5, 4477. |
| NiFe/nickel foam         | 400         | 0.1M KOH    | 0.075 s$^{-1}$ | Nat. Commun. 2015, 6, 6616. |
| CoFe$_2$O$_4$/C          | 300         | 1M KOH      | 0.0915 s$^{-1}$ | Adv. Mater. 2017, 29, 1604437. |
| Fe-based MOFs            | 400         | 0.1M KOH    | 0.03 s$^{-1}$ | Angew. Chem., Int. Ed. 2018, 57, 9660. |
| Fe, Co-based MOFs        | 300         | 0.1M KOH    | 0.27~1.82 s$^{-1}$ | J. Am. Chem. Soc., 2017, 139, 1778. |
| NiFe LDH                 | 300         | 1M KOH      | 0.13 s$^{-1}$-0.71 s$^{-1}$ | Adv. Mater. 2019, 1804769 |
| NiFe-LDH/C               | 300         | 1M KOH      | 0.3 s$^{-1}$ | Adv. Mater. 2017, 1705106 |
| FeCoW                    | 300         | 0.1M KOH    | 0.17~0.46 s$^{-1}$ | Science, 2016, 352, 333. |
| NiFe-LDH                 | 324         | 0.1M KOH    | 0.056 s$^{-1}$ | Small Methods 2018, 1800083 |
| NiFeN/C                  | 350         | 1 M KOH     | 0.46 s$^{-1}$ | Adv. Funct. Mater. 2018, 1706018 |
| DC+HHT                   | 370         | 0.1M KOH    | 0.276 s$^{-1}$ | This work                  |
Figure S16. (a) CV obtained with T-HHT loaded glassy carbon electrodes in the capacitance current range (1.02 V ~ 1.12V vs. RHE) at scan rates of 5, 10, 25, 50, 100, 200 and 400 mV, respectively. (b) The cathodic (red triangle) and anodic (blue circle) capacitance currents measured at 1.07 V vs. RHE plotted as a function of scan rate. The double-layer capacitance determined from this system is taken from the average of the absolute value of anodic and cathodic slopes of the linear fits.

Here, the $C_{dl}$ value of T-HHT measured by the scan rate dependent CVs is 0.0094 mF. By using equation 2, the ECSA value of T-HHT is calculated to be about 0.494 cm$^2$. 
Figure S17. (a) CV obtained with AT-supported HHT loaded glassy carbon electrodes in the capacitance current range (1.02 V ~ 1.12V vs. RHE) at scan rates of 5, 10, 25, 50, 100, 200 and 400 mV, respectively. (b) The cathodic (red triangle) and anodic (blue circle) capacitance currents measured at 1.07 V vs. RHE plotted as a function of scan rate. The double-layer capacitance determined from this system is taken from the average of the absolute value of anodic and cathodic slopes of the linear fits.

Here, The $C_{dl}$ value of AT-supported HHT measured by the scan rate dependent CVs is 0.0135 mF. By using equation 2, the ECSA value of AT-supported HHT is calculated to be about 0.709 cm$^2$, that is, the $\Delta$ECSA value of AT-supported HHT relative to H-HHT is 0.215 cm$^2$ (0.709-0.494=0.215).
Figure S18. (a) CV obtained with NT-supported HHT loaded glassy carbon electrodes in the capacitance current range (1.02 V ~ 1.12V vs. RHE) at scan rates of 5, 10, 25, 50, 100, 200 and 400 mV, respectively. (b) The cathodic (red triangle) and anodic (blue circle) capacitance currents measured at 1.07 V vs. RHE plotted as a function of scan rate. The double-layer capacitance determined from this system is taken from the average of the absolute value of anodic and cathodic slopes of the linear fits.

Here, The $C_{dl}$ value of NT-supported HHT measured by the scan rate dependent CVs is 0.0173 mF. By using equation 2, the ECSA value of NT-supported HHT is assessed to be 0.909 cm$^2$, that is, the ΔECSA value of NT-supported HHT relative to H-HHT is 0.415 cm$^2$ (0.909-0.494=0.415).
Figure S19. (a) CV obtained with DC-supported HHT loaded glassy carbon electrodes in the capacitance current range (1.02 V ~ 1.12V vs. RHE) at scan rates of 5, 10, 25, 50, 100, 200 and 400 mV, respectively. (b) The cathodic (red triangle) and anodic (blue circle) capacitance currents measured at 1.07 V vs. RHE plotted as a function of scan rate. The double-layer capacitance determined from this system is taken from the average of the absolute value of anodic and cathodic slopes of the linear fits.

Here, the $C_{dl}$ value of DC-supported HHT measured by the scan rate dependent CVs is 0.0187 mF. By using equation 2, the ECSA value of DC-supported HHT is calculated to be about 0.984 cm$^2$, that is, the $\Delta$ECSA value of DC-supported HHT relative to H-HHT is 0.49 cm$^2$ (0.984-0.494=0.49).
Figure S20. Electrochemical activities of supported OLC catalysts for OER.
Figure S21. The net contents of AT molecules on supported OLC catalyst with TG measurement.
Figure S22. (a-b) CV obtained with (a) pure OLC and (b) AT-supported OLC loaded glassy carbon electrodes in the capacitance current range (1.02 V ~ 1.12V vs. RHE) at scan rates of 5, 10, 25, 50, 100, 200 and 400 mV, respectively. (c-d) The cathodic (red triangle) and anodic (blue circle) capacitance currents measured at 1.07 V vs. RHE plotted as a function of scan rate. The double-layer capacitance determined from this system is taken from the average of the absolute value of anodic and cathodic slopes of the linear fits.

Here, the $C_{dl}$ values of pure OLC and AT-supported OLC measured by the scan rate dependent CVs are 0.112 mF and 0.178 mF, respectively. By using equation 2, the ECSA values of pure OLC and PQ-modified OLC are assessed to be 5.89 cm$^2$ and 9.36 cm$^2$, respectively.
Figure S23. Possible required reaction energies of OH⁻ at different carbon positions (α-, β- and γ) in the first OER process.