

Article

Supplementary Materials: Terpyridine-Containing Imine-Rich Graphene for the Oxygen Reduction Reaction

Min Seok Lee ¹, Mun Ho Yang ¹, Jong S. Park ² and Dong Wook Chang ^{1,*}

¹ Department of Industrial Chemistry, Pukyong National University, Busan 48547, Korea; lms@pknu.ac.kr (M.S.L.); ymh@pknu.ac.kr (M.H.Y.)

² Department of Organic Material Science and Engineering, Pusan National University, Busan 46241, Korea; jongpark@pnu.ac.kr

* Correspondence: dwchang@pknu.ac.kr; Tel.: +82-51-629-6444

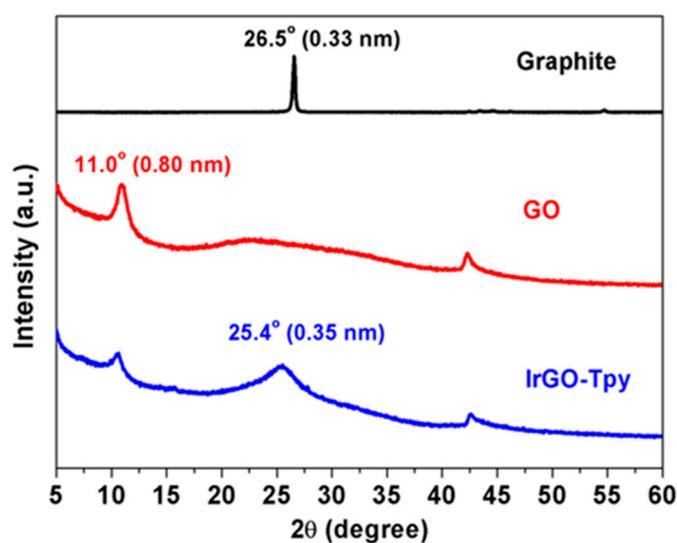


Figure S1. XRD diffraction patterns of graphite, GO, and IrGO-Tpy with *d*-spacing.

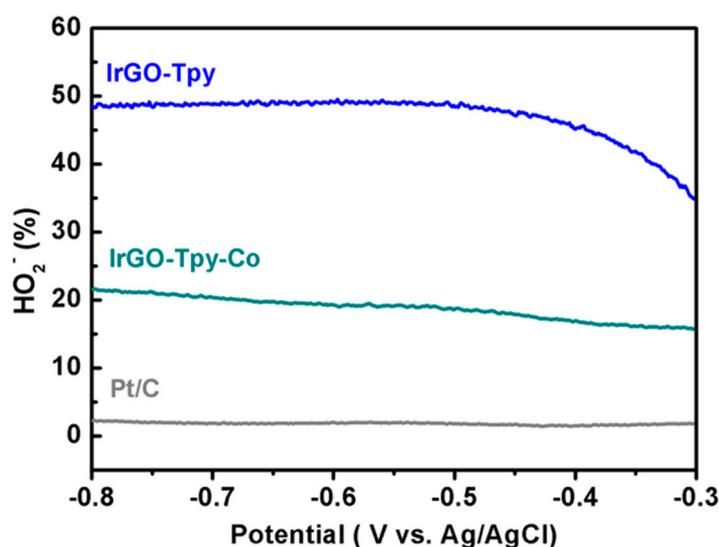


Figure S2. Peroxide percentages of IrGO-Tpy, IrGO-Tpy, and Pt/C as a function of the electrode potential at 1600 rpm.

Calculation of electron transferred number (n)

The kinetic analysis for ORR was conducted according to Koutecky-Levich plots:

$$\frac{1}{j} = \frac{1}{j_k} + \frac{1}{B\omega^{0.5}} \quad (1)$$

where j_k is the kinetic current and B is Levich slope which is given by:

$$B = 0.2nF(D_{O_2})^{2/3}\nu^{-1/6}C_{O_2} \quad (2)$$

The constant 0.2 is generally adopted when the rotation speed is expressed in rpm. n is the number of electrons transferred for the reduction of one O_2 molecule, F is the Faraday constant ($F = 96485 \text{ C/mol}$), D_{O_2} is the diffusion coefficient of O_2 ($D_{O_2} = 1.9 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$), ν is the kinematics viscosity for KOH ($\nu = 0.01 \text{ cm}^2 \text{ s}^{-1}$) and C_{O_2} is concentration of O_2 in the solution ($C_{O_2} = 1.2 \times 10^{-6} \text{ mol cm}^{-3}$).

According to equations (1) and (2), the number of electrons transferred (n) can be obtained from the slope of Koutecky-Levich plot of j^{-1} vs. $\omega^{-1/2}$.

Calculation of electron transferred number (n) and the yield of peroxide (HO_2^-) by rotating ring disk electrode (RRDE)

The number of electron transferred (n);

$$n = \frac{(4 \times I_d)}{(I_d \times \frac{I_r}{N})} \quad (3)$$

Where I_r and I_d are the current obtained from the ring and disk electrode, respectively.

N is the current collection efficiency of Pt ring electrode and is determined to be 0.424 using the redox reaction of $K_3Fe(CN)_6$.

The yield of hydrogen peroxide;

$$\%HO_2^- = \frac{(200 \times \frac{I_r}{N})}{(I_d \times \frac{I_r}{N})} \quad (4)$$

Table S1. Elemental analyses of graphite, GO and IrGO-Tpy.

Materials	C	O	H	N	Sum	C/O	C/N
Graphite	98.74	BDL ^a	0.11	BDL ^a	98.85	∞^b	∞^b
GO	53.19	42.10	2.30	BDL ^a	97.59	1.68	∞^b
IrGO-Tpy	76.17	11.54	2.59	6.45	96.75	8.80	13.78

^aBDL = Below detection limit

^b ∞ = Unlimited

Table S2. Elemental compositions of IrGO-Tpy and IrGO-Tpy-Co obtained from XPS analysis.

Materials	C	O	N	Co	Cl	Sum
IrGO-Tpy	85.59	8.95	5.47	BDL ^a	BDL ^a	100.00
IrGO-Tpy-Co	82.66	9.54	6.26	0.73	0.81	100.00

^aBDL = Below detection limit

Table S3. Onset potentials and current densities at -0.5 V of all samples on a rotating disk electrode at a rotation speed of 1600 rpm and a scan rate of 10 mVs⁻¹

Sample	Onset Potential (V)	Current Density (mA/cm ²) at -0.6 V
IrGO-Tpy	-0.18	-2.71
IrGO-Tpy-Co	-0.11	-3.80
Pt/C	-0.01	-5.18

Table S4. Electron transferred numbers (n) of all samples from K-L plots and RRDE measurements at different electrode potentials of -0.40 V, -0.50 V and -0.60 V.

Sample	K-L equation ^a			RRDE ^b		
	-0.40 V	-0.50 V	-0.60 V	-0.40 V	-0.50 V	-0.60 V
IrGO-Tpy	2.95	2.90	2.97	3.10	3.03	3.02
IrGO-Tpy-Co	3.73	3.73	3.72	3.66	3.63	3.62
Pt/C	4.00	3.97	3.94	3.97	3.96	3.96

^aCalculated by the equation of $\frac{1}{j} = \frac{1}{j_k} + \frac{1}{B\omega^{0.5}}$, $B = 0.2nF(D_{O_2})^{2/3}v^{-1/6}C_{O_2}$

^bCalculated by the equation of

$$n = \frac{(4 \times I_d)}{(I_d \times \frac{I_r}{N})} \quad (5)$$



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