

## Supporting Information

### Mechanistic Insights into the Visible Light Photocatalytic Activity of g- C<sub>3</sub>N<sub>4</sub>/Bi<sub>2</sub>O<sub>2</sub>CO<sub>3</sub>-Bi<sub>4</sub>O<sub>7</sub> Composites for Rhodamine B Degradation

Aleena Majeed<sup>a</sup>, Samna Hassan<sup>a</sup>, Musarrat Zahra<sup>a</sup>, Iqra Rafique<sup>b</sup>, Sajid Iqbal<sup>c</sup>, Munib Ahmad Shafiq<sup>d</sup>, Rashid Nazir Qureshi<sup>d</sup>, Ramzan Akhtar<sup>e</sup>, Muhammad Rehan<sup>f</sup>, Mohsin Ali Raza Anjum<sup>e</sup>, Sheeraz Mehboob<sup>e</sup>, Jaweria Ambreen<sup>a,g\*</sup>, Jae Ho Yun<sup>h\*</sup>, Muhammad Saifullah<sup>e\*</sup>

<sup>a</sup>Department of Chemistry, COMSATS University Islamabad, Park Road, 45550, Islamabad, Pakistan.

<sup>b</sup>Isotope Production Division (IPD), Pakistan Institute of Nuclear Science and Technology (PINSTECH), P.O.Box 45650, Nilore Islamabad, Pakistan.

<sup>c</sup>Department of Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology, Daejeon, South Korea.

<sup>d</sup>Central Analytical Facility Division (CAFD), Pakistan Institute of Nuclear Science and Technology (PINSTECH), Islamabad, Pakistan.

<sup>e</sup>Chemistry Division, Pakistan Institute of Nuclear Science and Technology (PINSTECH), Islamabad, Pakistan.

<sup>f</sup>Photovoltaic Research Department, Korea Institute of Energy Research (KIER), Daejeon, South Korea.

<sup>g</sup>Department of Biomedical Engineering & Health Sciences, Faculty of Electrical Engineering, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Johor, Malaysia.

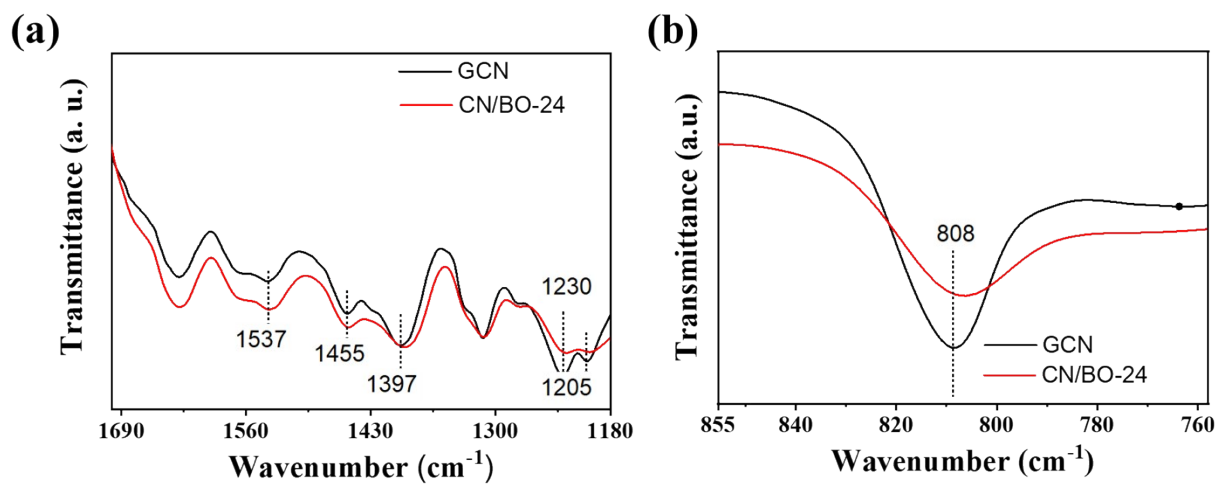
<sup>h</sup>Department of Energy Engineering, Korea Institute of Energy Technology, South Korea.

Corresponding authors:

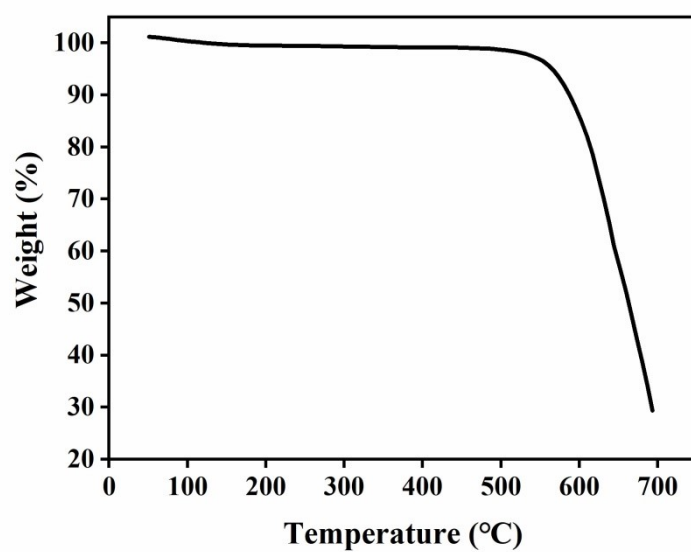
Jaweria Ambreen ([Jaweria.ambreen@comsats.edu.pk](mailto:Jaweria.ambreen@comsats.edu.pk))

Jae Ho Yun ([jhyun@kentech.ac.kr](mailto:jhyun@kentech.ac.kr))

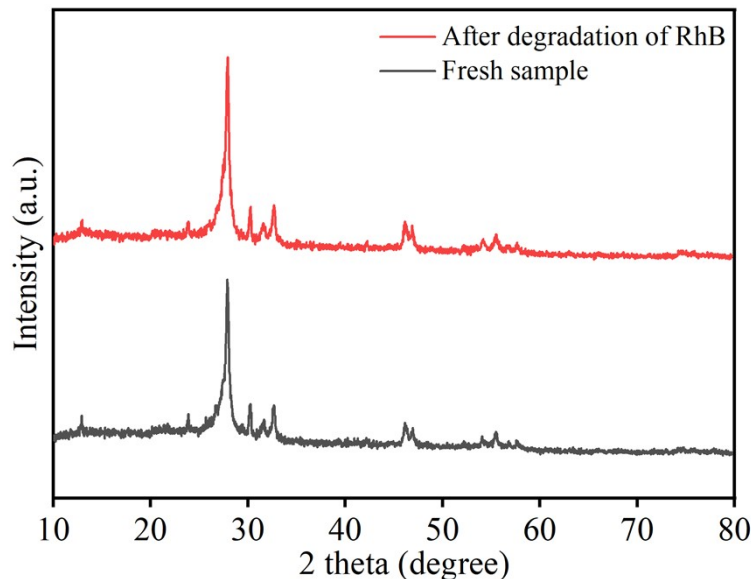
Muhammad Saifullah ([Saifi.551@gmail.com](mailto:Saifi.551@gmail.com))



**Fig. S1:** FTIR patterns of GCN and CN/BO-24 in the wavenumber range of (a) 1180 to 1700  $\text{cm}^{-1}$  and (b) 758 to 855  $\text{cm}^{-1}$ .



**Fig. S2:** Thermogravimetric analysis curve of g-C<sub>3</sub>N<sub>4</sub> (GCN).



**Fig. S3:** XRD patterns of the CN/BO-24 sample, freshly prepared and after RhB photocatalytic degradation.

### Electrochemical experiment details

Catalyst ink is prepared by sonicating 10 mg of catalyst in a mixture of 1 mL of deionized water and ethanol each (1:1), and 20  $\mu\text{L}$  of Nafion solution (5%) in a beaker. The working electrode is prepared by drop casting of catalyst suspension on 7 mm x 6 mm graphite felts. After the drop casting step, the electrode is dried by heating it at 80  $^{\circ}\text{C}$ , and the catalyst loading is maintained at  $\approx 20 \text{ mg}/\text{cm}^2$  for each electrode. The obtained performance curve versus the Ag/AgCl reference electrode is converted to RHE using the following equation:

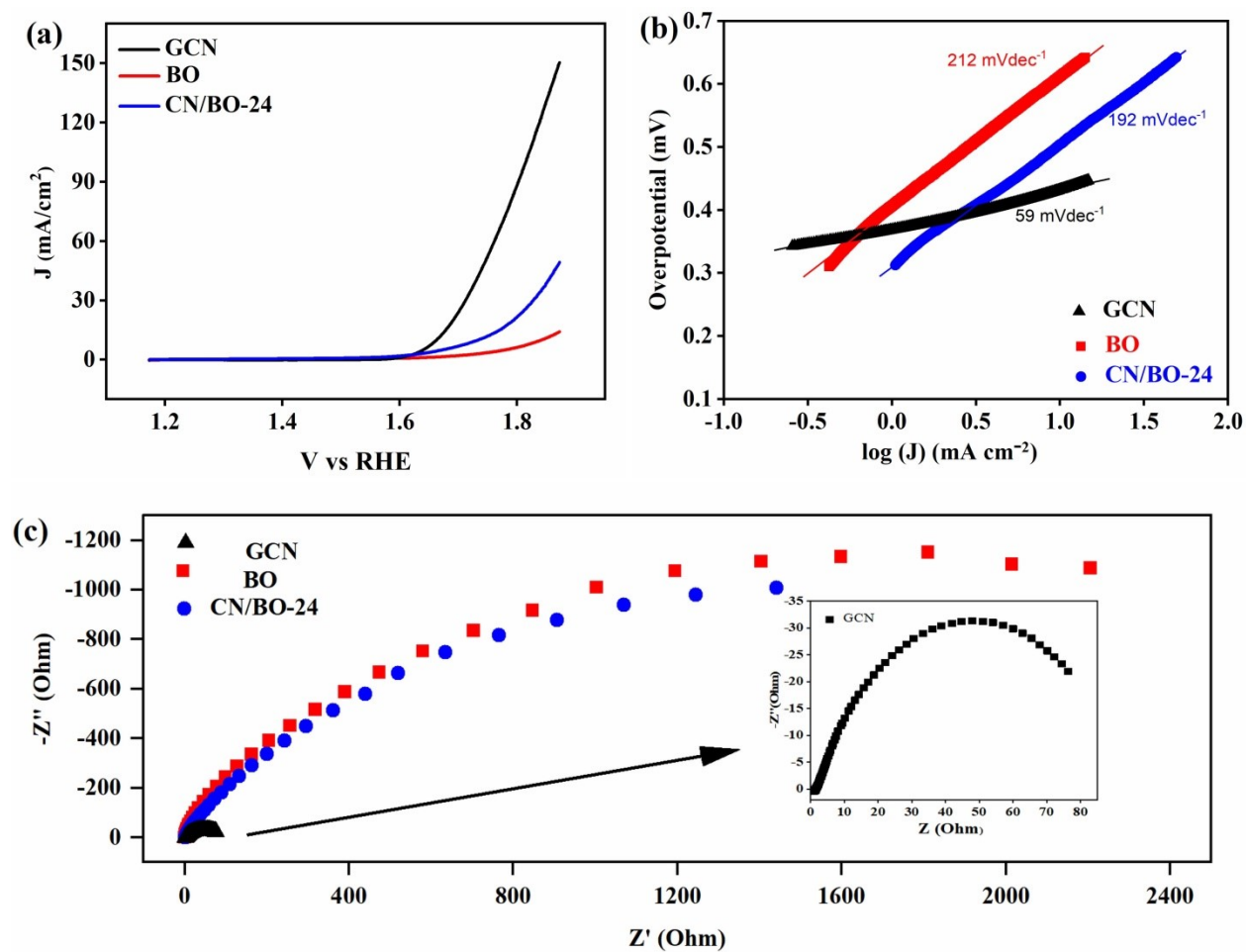
$$E_{\text{RHE}} = E_{\text{Ag/AgCl}} + E^{\circ}_{\text{Ag/AgCl}} + 0.0591 \times \text{pH}$$

where  $E_{\text{RHE}}$  is the potential vs. RHE,  $E_{\text{Ag/AgCl}}$  is the measured potential vs. the Ag/AgCl electrode,  $E^{\circ}_{\text{Ag/AgCl}}$  is the standard potential of the Ag/AgCl electrode.<sup>1</sup>

The performance for the oxygen evolution reaction (OER) is assessed in alkaline media (1.0 M KOH) using a three-electrode setup, Ag/AgCl as the reference electrode, platinum wire as the counter electrode, and the above-prepared graphite felt as a working electrode. The electrocatalytic OER performance of GCN, BO, and CN/BO-24 working electrodes is evaluated by linear sweep voltammetry (LSV) at a scan rate of 5  $\text{mV s}^{-1}$ , as shown in Fig. S2(a). The GCN displays the best OER activity and displays overpotential value ( $\eta_{10} = 430 \text{ mV}$ ) for current

density (J) of 10 mA cm<sup>-2</sup>, which is lower than CN/BO-24 (500 mV) and pristine BO (610 mV), respectively.

The reaction mechanism & kinetics of electrodes are determined by Tafel analysis, a plot between overpotential and log (J), as shown in Fig. S2(b). The pristine GCN exhibits a lower Tafel slope of 59 mV dec<sup>-1</sup>, in contrast to the pristine BO (192 mV dec<sup>-1</sup>) and CN/BO-24 composite (212 mV dec<sup>-1</sup>). This indicates that all electrodes follow the Volmer–Heyrovsky mechanism in alkaline media. Moreover, a low Tafel slope of GCN indicates a fast reaction rate as compared to both pristine BO and the CN/BO-24 composite. Electrochemical impedance studies (EIS) are also carried out to assess the charge transfer resistance at the electrode-electrolyte interface. As shown in the Nyquist plots (Fig. S2(c)), the GCN has much lower charge transfer resistance in comparison to both pristine BO and CN/BO-24. From the above results, it can be concluded that the pristine GCN displays better electrochemical performance for OER, while the CN/BO-24 composite shows a good photocatalytic performance due to the suitable band alignments between the constituent elements.



**Fig. S4:** OER study of GCN, BO, and CN/BO-24 catalysts, (a) LSV Analysis, (b) Tafel plots, and (c) Nyquist plot obtained from EIS analysis.

### ***Reference***

1. C. Lai, S. Ji, H. Zhou, L. Ma, H. Wang, J. Hu, J. Sun, K. Zhang, X. Liu and F. Li, *Available at SSRN 3996836*, 2022.