Supplementary Information (SI) for Journal of Materials Chemistry C.

SUPPORTING INFORMATION

A Field-Deployable Multimodal Device Integrated with Paper Strips and LIG Platforms for Rapid Optical-Electrochemical Detection of Organophosphate Nerve Agent Simulants

Rikitha S Fernandes,[a] Ritesh Kumar Singh,[b] Sanket Goel,[b] and Nilanjan Dey,[a]*
[a]Department of Chemistry, Birla Institute of Technology and Science Pilani, Hyderabad Campus, Hyderabad 500078, India
[b]Department of Department of Electrical & Electronics Engineering, Birla Institute of Technology
*Email: nilanjandey.iisc@gmail.com, nilanjan@hyderabad.bits-pilani.ac.in

EXPERIMENTAL SECTION

1.1 General: All solvents, reagents, and chemicals were obtained from reputable chemical suppliers and were used as received without further purification. Solvents were distilled and dried prior to use. FTIR spectra were acquired on a Perkin-Elmer Spectrum BX FT-IR system and are reported in wavenumbers (cm^{-1}). ^1H and ^{13}C NMR spectra were recorded on a Bruker Avance Neo 400 spectrometer, operating at 400 MHz and 100 MHz, respectively. Chemical shifts are reported in ppm relative to tetramethylsilane (TMS) as an internal standard. Mass spectra were obtained using a Shimadzu LCMS 8040 system

1.2 Spectroscopic studies. UV-Vis spectroscopic measurements were conducted using a JASCO V-650 UV-Vis spectrophotometer with a slit width of 5 nm. Sensing experiments were performed by adding the required amounts of ascorbic acid (1% DMSO) to aqueous solutions of probe **1**. Fluorescence measurements were carried out using a FluoroLog-TM (Horiba Scientific) spectrofluorometer, with slit widths set at 5 nm for both excitation and emission and an excitation wavelength of 500 nm.

Analytes (1-9): $POCl_3$, AcOH, TEA (Triethylamine), TMP (Trimethyl Phosphate), $SOCl_2$, DCNP (Diethyl Cyanophosphate), DMMP (Dimethyl Methylphosphonate), DCP (Diethyl Chlorophosphate), Na_2HPO_4

1.3 Lifetime measurements: Lifetime measurements were performed using Horiba Delta flex Modular fluorescence lifetime system with the following instrumental parameters: 510 nm NanoLED excitation source with an instrument response function of about 165 ps, and peak preset 10000 counts.

1.5 ^{1}H NMR Studies. ^1H NMR titration studies of compound **1** (5 mM) were performed with DCP (1.0 equiv) in DMSO-d_6. The spectra were recorded using identical parameters.

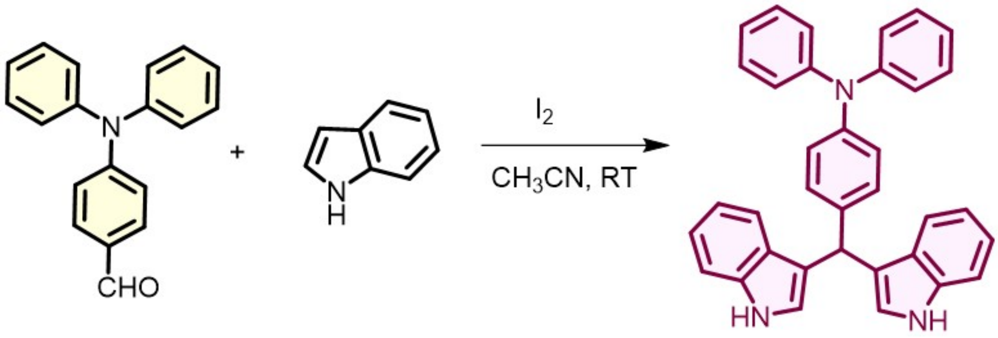
1.6 Scanning Electron Microscopy (SEM): Samples for SEM analysis were drop-cast onto a silicon wafer at the desired concentrations, followed by overnight solvent evaporation. The silicon wafer was subsequently sputter-coated using a Leica Ultra Microtome EM UC7. The prepared stubs were then imaged at 1 μm/500 nm magnification using an FEI Apreo LoVac.

1.7 Dynamic Light Scattering (DLS) Study: Zetasizer Nano S (Malvern Instruments) at 25 °C was used for DLS analysis. Probe **1** in the absence and presence of DCP was recorded. Before recording, the samples were mixed thoroughly to obtain a consistent suspension in water.

SYNTHESIS AND CHARACTERIZATION

Synthesis of compound **1**

Compound 1 was synthesised following established protocols in the literature. Briefly, Triphenylamine aldehyde (0.5 mmol) was dissolved in acetonitrile (2 mL) and stirred, to which indole (2 equiv.) was added alongside a catalytic amount of I_2 (0.05 equiv.). The mixture was vigorously stirred at room temperature for 30 minutes. The obtained product was purified by column chromatography using a hexane/ethyl acetate (9:1) solvent system. Yield: 90%. ^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 10.80 (s, 2H), 7.33 (d, J = 8.1 Hz, 2H), 7.29 (d, J = 8.4 Hz, 4H), 7.27 – 7.22 (m, 4H), 7.03 (dd, J = 7.0, 1.0 Hz, 2H), 7.01 – 6.97 (m, 2H), 6.97 – 6.95 (m, 2H), 6.94 (d, J = 1.0 Hz, 2H), 6.93 – 6.90 (m, 2H), 6.89 – 6.84 (m, 4H), 5.78 (s, 1H).



Scheme S1: Synthetic scheme of probe **1**

ADDITIONAL SPECTROSCOPIC DATA

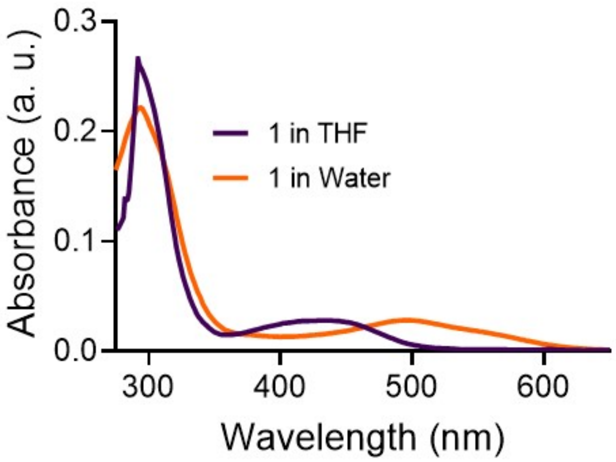


Figure. **S1** UV-Visible spectra of probe **1** (10 μM) in THF and water

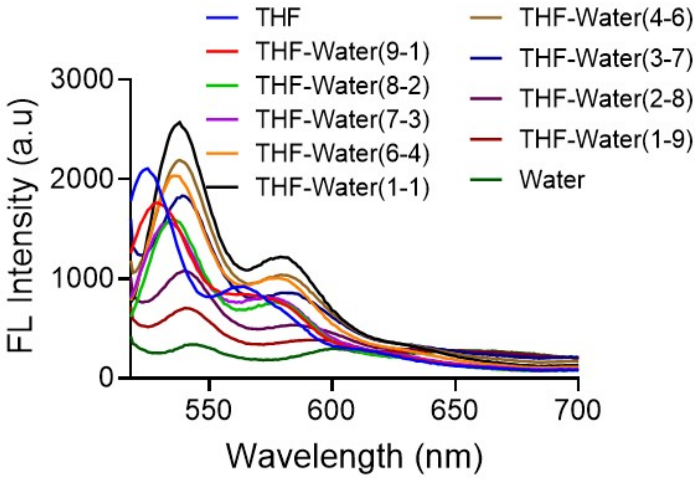


Figure. S2 Fluorescence spectra of probe **1** (10 μM, λ_{ex} = 500 nm) in different THF: water mixture medium.

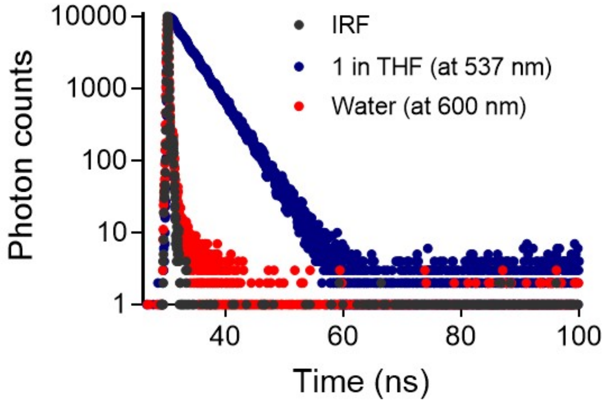


Figure. **S3** Fluorescence lifetime of probe **1** (10 µM, λ_{ex} = 500 nm) in THF and water medium

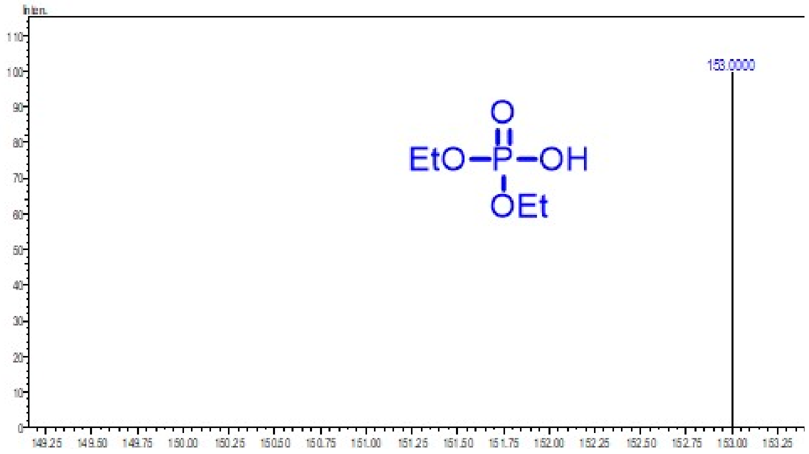


Figure. **S4** Mass spectrometry analysis of 1. DCP mixture

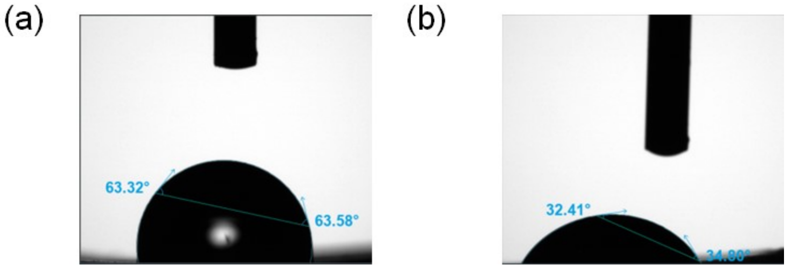


Figure. **S5** Contact angle measurement of (a) Bare LIG and (b) Modified LIG

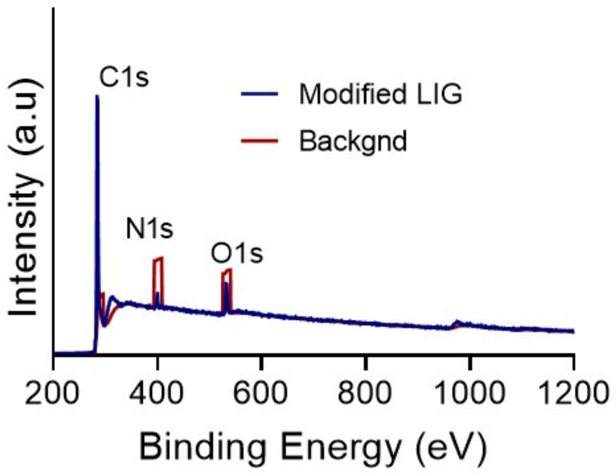


Figure. **S6** XPS survey spectra of modified LIG

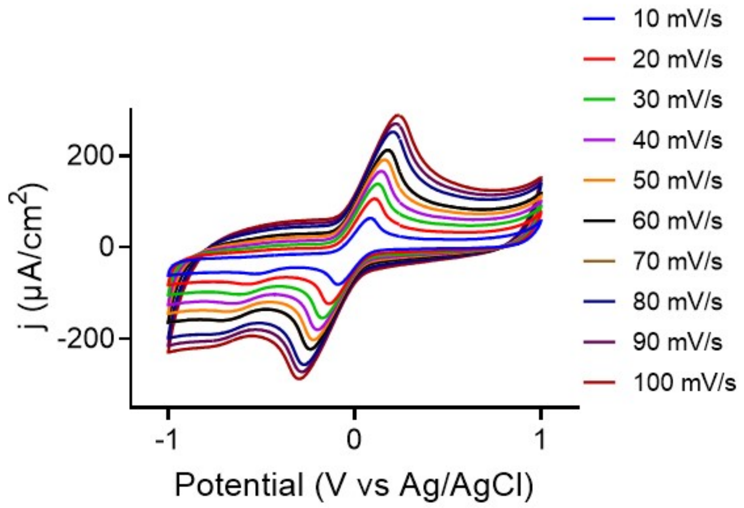


Figure. **S7** Cyclic voltammogram of modified LIG with the potassium ferricyanide-KCl solution for different scan rates (10-100 mV/s) in 0.1 M TBAP in CH_3CN solution.

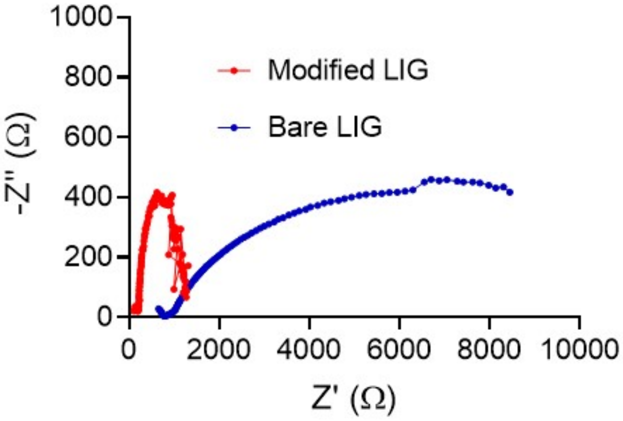


Figure. **S8** EIS of bare LIG and modified LIG

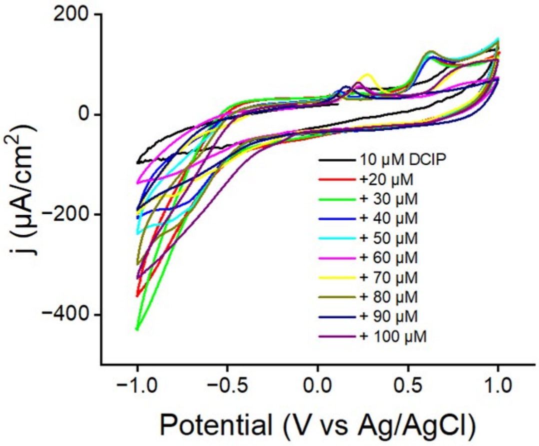


Figure. **S9** Cyclic voltammogram of modified LIG in the presence of DCP (0-100 μM) at 50 mV/s scan rate in 0.1 M TBAP in CH_3CN solution.