

## Supporting Information

### **Novel concept and design for Highly efficient photo electrocatalytical performance and stable charges Properties Material: Green Development of a Next-Generation Technology Innovation**

Abdul Qayoom Mugheri<sup>a</sup> & <sup>f\*</sup>, Kashif Ali<sup>b</sup>, Ali Asghar sangah<sup>c</sup>, Mazhar Iqbal khaskheli<sup>d</sup> Muhammad Younis Laghari<sup>e</sup>, Nadeem Ahmed Mugheri<sup>a</sup>, Muhammad Rajib Soomro<sup>a</sup>, *Muhammad Ishfaq Chohan<sup>a</sup>* Arsalan Ahmed Mugheri<sup>a</sup>, Aftab Kandhro<sup>a</sup>

<sup>a</sup>Dr. M.A Kazi Institute of Chemistry University of Sindh Jamshoro, 76080, Sindh Pakistan

<sup>b</sup>Hunan Key Laboratory for Super Microstructure and Ultrafast Process, School of Physics and Electronics, Central South University, Changsha 410083, China

<sup>c</sup>Department of Basic Sciences and Related Studies, Mehran University of Engineering and Technology, Jamshoro, 76080, Pakistan

<sup>d</sup>Department of Chemistry GC University Hyderabad

<sup>e</sup>The Department of Fisheries and Aquatic Sciences University of Sindh Jamshoro, 76080, Sindh Pakistan

<sup>ef</sup>National center of excellence in Analytical Chemistry University of Sindh Jamshoro, 76080, Sindh Pakistan

\*Corresponding author: Abdul Qayoom Mugheri, PhD

Email

address: [a.qmugheri87@gmail.com](mailto:a.qmugheri87@gmail.com)

### **Methods**

Chemicals: Ni, Co and ZnO nanoparticles were synthesized and dispersed in ethanol following a reported method [1]. 2-ethylhexyl)-3,9-diundecyl-12,13-dihydro, thiazolo, thieno, pyrrolo, indole-2,10-diyl, methanylylidene, 5,6-difluoro-3-oxo 2,3-dihydro-1H-indene-2,1-diylylidene, dimalononitrile, polyethylhexyl-3-fluoro, benzo, dithiophene, 2-ethylhexyl, and benzo dithiophene-4,8-dione.

## Photoanode fabrication

The film samples were excited with a suitable light source, and the emitted light was collected and analyzed. By examining the PL spectra, researchers can gain valuable information about the optical properties of materials, such as the bandgap energy, the presence of impurities or defects, the emission efficiency, and the nature of excitonic transitions. This information is crucial for understanding and optimizing the performance of materials in various applications, including optoelectronics, photovoltaics, displays, sensors, and lighting technologies. The absorption spectra were measured to study the absorption characteristics of the film. This information helps to determine the wavelength range at which the film can absorb light. The spectroscopic analyses mentioned in the passage are commonly used to characterize the optical properties of materials, such as semiconducting film. ITO substrates were cleaned by deionized water, ethanol, sequentially. Metal oxides (Ni, Co, Zn) nanoparticles were spin-coated twice on the ITO substrates in air. Dithiophene-4,8-dione/Dimalononitrile blend solution (1.2:1 weight ratio, 18 mg mL<sup>-1</sup> in chloronaphtalene) were spin-coated on the metal oxide nanoparticles layer, then the film was annealed at 120 °C for 120 s. To deposit the dithiophene-4,8-dione film on the dithiophene-4,8-dione/Dimalononitrile, the dithiophene-4,8-dione film was fabricated by dropping (18 mg mL<sup>-1</sup> in chlorobenzene) on the deionized water contained in a petri dish. They provide valuable insights into the energy band structure, absorption, and emission behavior of the materials. It's worth noting that the specific details and results of the spectroscopic analyses mentioned in the passage are not provided, so further information would be required to discuss the specific findings and implications of the measurements were obtained.

**Spectroscopic analyses** The absorption spectra were collected using a UV-visible (UV-Vis) spectrometer manufactured by Agilent Technologies, specifically the Cary 60 model. The steady-state photoluminescence (PL) spectra were recorded using a custom-built system consisting of several components. For excitation, a collimated Laser Diode Module (CPS532) from THORLABS emitting light at a wavelength of 532 nm was used as the light source. This laser diode module provided the necessary energy to excite the materials and induce photoluminescence. To calibrate and measure the absolute intensity of the emitted light, an AvaLight-CAL-Mini instrument was used. This instrument helps ensure accurate measurements of the emitted light intensity during the PL spectroscopic analysis. By using this setup, were able to obtain absorption

spectra and steady-state PL spectra, which provide information about the absorption and emission properties of the materials.

**Transient absorption spectroscopy** In the study, transient absorption spectroscopy was performed using a Helios spectrometer manufactured by Spectra. This technique allows for the measurement of broadband pump-probe femtosecond transient absorption spectra and kinetics for thin film samples. To generate the ultrafast laser pulses needed for the experiments, a 1 kHz was used, producing laser pulses at a wavelength of 800 nm with a duration of 100 femtoseconds (fs). A portion of the 800 nm pulse was directed to an optical parametric amplifier and a frequency mixer to tune the visible pump pulses at various wavelengths. The pump pulses were modulated at a frequency of 500 Hz using a mechanical chopper. The remaining portion of the 800 nm pulse was sent to a mechanical delay stage with a time window of 6 nanoseconds (ns). From there, it was directed through a non-linear crystal to generate a white light probe spanning the wavelength range of 400 to 1600 nm. The probe pulse was split into two parts using a neutral density filter. One part served as the reference and was directly sent to fiber-optic coupled multichannel spectrometers. The other part of the probe pulse, along with the pump pulse, was focused onto the same spot on the thin film samples, with a beam size of approximately 0.5 mm<sup>2</sup>, before being directed to the spectrometer. To compensate for fluctuations, the measured spectrum was normalized to the reference spectrum and averaged over several scans to achieve a good signal-to-noise ratio. Data analysis was performed using the commercialized Surface. This experimental setup enabled to properly investigate the dynamics of the thin film samples through transient absorption spectroscopy, providing valuable information about their excited-state dynamics and photoinduced processes on femtosecond timescales.

**Photoinduced absorption spectroscopy** In the study, photoinduced absorption (PIA) spectroscopy was performed using a modified microsecond–second transient absorption (TA) spectroscopy setup. PIA analysis allows for the investigation of photoinduced changes in the absorption properties of a material. The excitation source used in the PIA analysis was a high-power LED (LEDENGIN) emitting light at a wavelength of 365 nm. The LED was driven by a high-precision DC power supply to provide the required excitation energy. To direct the LED light to the sample, a liquid light guide was used. Light pulses for the experiments were generated using a MOSFET transistor, with the gate of the transistor being modulated by a data acquisition (DAQ).

The DAQ card was responsible for controlling the timing and modulation of the excitation pulses. Importantly, all data were sampled without prior amplification using the DAQ card. The excitation fluences, which measure the energy density of the incident light, were measured using a digital power meter and a silicon photodiode power sensor. This allowed for accurate determination of the energy delivered to the sample during the PIA experiments. The photoelectrochemical cell configuration used for PIA analysis was the same as described in the subsequent section of the study. By employing this modified TA spectroscopy setup, the to investigate photoinduced absorption changes in the material under study, providing insights into the excited-state dynamics and optical properties of the sample.

### **Photoelectrochemical characterization:**

In the photoelectrochemical characterization of organic photoanodes, a cappuccino cell was used. A cappuccino cell is a compact chamber made from polyether ether ketone (PEEK) and typically features a small light window to allow for illumination of the working electrode. The cappuccino cell provides a controlled environment for performing photoelectrochemical measurements. The three-electrode configuration was employed in the cappuccino cell. The three electrodes used. Using this three-electrode configuration, the organic photoanode's photoelectrochemical behavior can be studied by applying an appropriate bias voltage to the working electrode and measuring the resulting photocurrent or other electrochemical parameters. The reference electrode and counter electrode ensure accurate measurements and provide a suitable electrochemical environment for the working electrode. It's worth noting that additional components or modifications specific to the experimental setup may be involved, but the information provided describes the essential elements of the photoelectrochemical characterization setup for organic photoanodes in the cappuccino cell. The electrolytes were 0.1 M Phosphate buffer (pH 8.5), LSV were recorded with the scan rate of 10 mV s<sup>-1</sup>, and the applied potential was controlled by an Auto lab potentiostat under AM 1.5G illumination calibrated by a silicon photodiode. Applied potentials versus the reference electrode. The operating area of the organic photoanode was 0.385 cm<sup>2</sup>. The external quantum efficiency (EQE) was measured using a xenon lamp coupled with a monochromator. EQE was calculated dividing photogenerated electron flux by incident photon flux, by measuring the photocurrent at the mono chromated light and the mono chromated light intensity at different wavelength. Accumulated hydrogen amounts are measured by the clark electrode. Theoretical

hydrogen amounts determined by dividing measured photogenerated charges by  $2F$ , where  $F$  is Faraday's constant,  $96500 \text{ C mol}^{-1}$  as shown in figure 5.

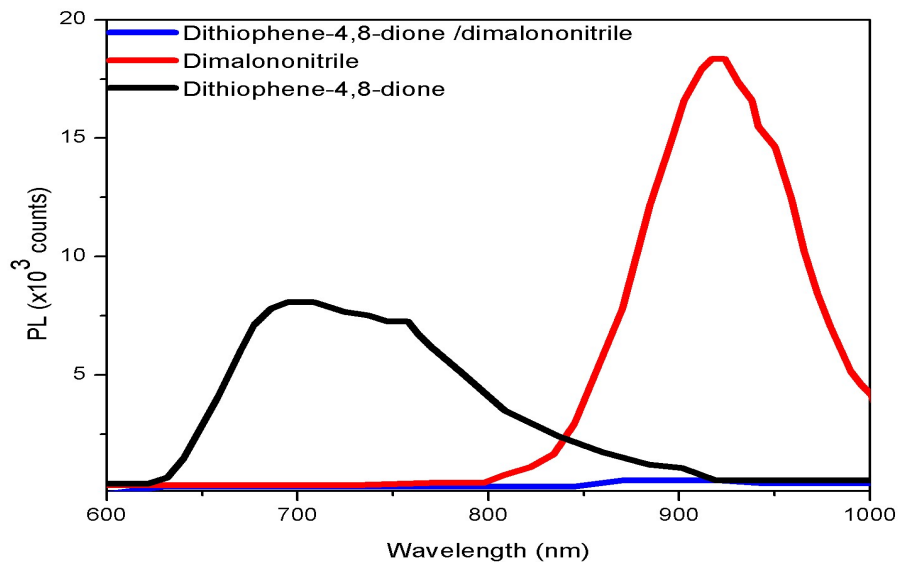


Figure S1. The photoluminescence spectra (normalized to absorbed photon amounts at 532 nm pump wavelength) of neat dithiophene-4,8-dione, dimalononitrile, and dithiophene-4,8-dione/dimalononitrile.

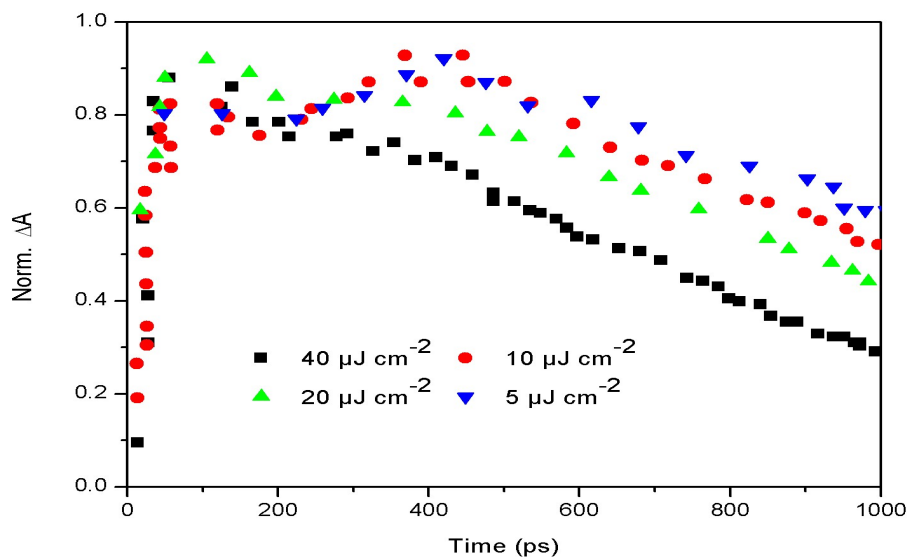


Figure S2. Absorption kinetics at normalized transient of dithiophene-4,8-dione/dimalononitrile

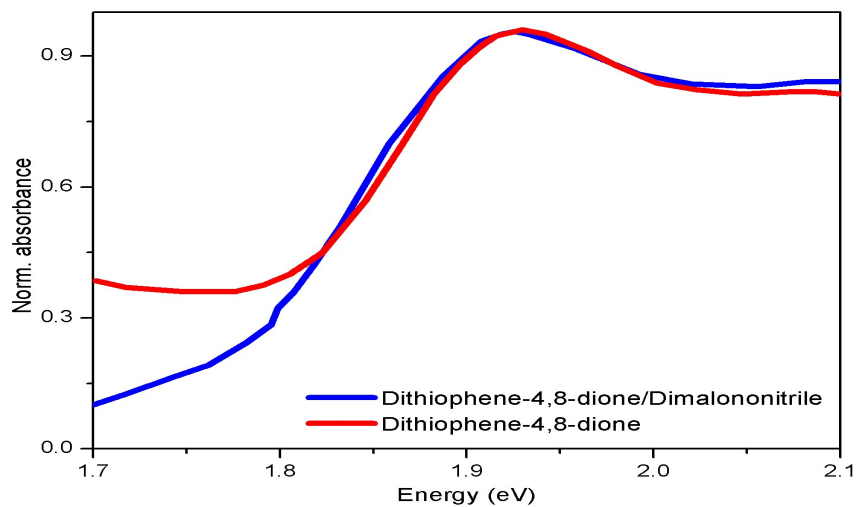
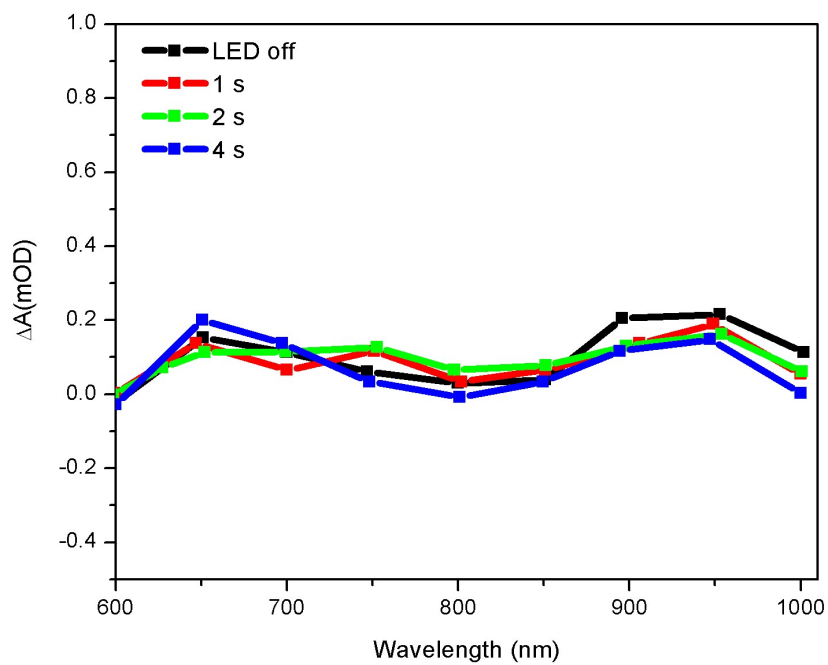


Figure S3. Normalized absorption spectra of dithiophene-4,8-dione/dimalononitrile and dithiophene-4,8-dione as a function of energy.



S4 Dithiophene-4,8-dione/dimalononitrile spectra on Photoinduced absorption (PIA)

1.W. Lee, J. Yeop, J. Heo, Y. J. Yoon, S. Y. Park, J. Jeong, Y. S. Shin, J. W. Kim, N. G. An, D. S. Kim, J. Park, J. Y. Kim, Sci. Rep. 2020, 10, 18055.