

Supplementary Material for

**Development of a Semiconducting Supramolecular Copper(II)-Metallogel for Antimicrobial and Microelectronic Device Applications**

Sangita Some,<sup>a</sup> Pubali Das,<sup>b</sup> Suchetana Pal,<sup>c</sup> Subhendu Dhibar,<sup>\*a</sup> Dimpal Kumari,<sup>d</sup> Subham Bhattacharjee,<sup>e</sup> Soumya Jyoti Ray,<sup>d</sup> Timothy O. Ajiboye,<sup>f</sup> Somasri Dam,<sup>\*c</sup> Partha Pratim Ray,<sup>\*b</sup> Bidyut Saha<sup>\*a</sup>

<sup>a</sup>Colloid Chemistry Laboratory, Department of Chemistry, The University of Burdwan, Golapbag, Burdwan-713104, West Bengal, India \*E-mail: sdhibar@scholar.buruniv.ac.in, Tel: +91 7001575909 (S. Dhibar); \*E-mail: bsaha@chem.buruniv.ac.in, Tel: +91 9476341691 (B. Saha).

<sup>b</sup>Department of Physics, Jadavpur University, Jadavpur, Kolkata-700032, India; \*E-mail: parthap.ray@jadavpuruniversity.in; Tel: +91 3324572844 (P. P. Ray).

<sup>c</sup>Department of Microbiology, The University of Burdwan, Burdwan-713104, West Bengal, India, \*E-mail: sdam@microbio.buruniv.ac.in (S. Dam).

<sup>d</sup>Department of Physics, Indian Institute of Technology Patna, Bihar-801106, India.

<sup>e</sup>Department of Chemistry, Kazi Nazrul University, Asansol-713303, West Bengal, India.

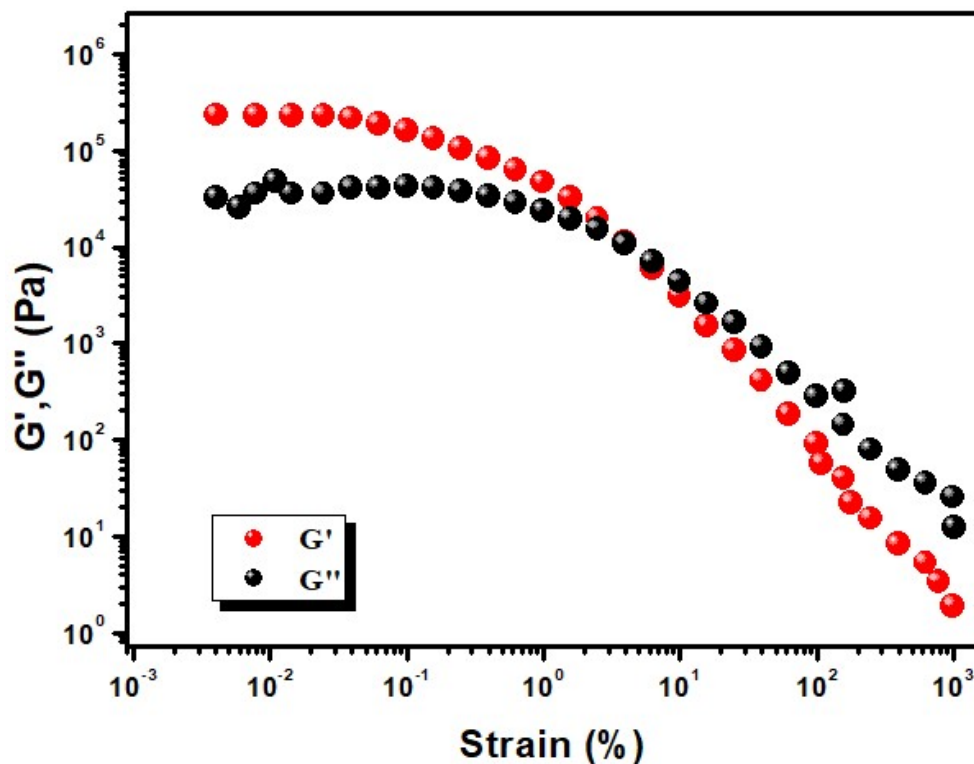
<sup>f</sup>Department of Chemistry, University of the Free State, Bloemfontein, 9301, South Africa.

## **Table of Content**

Rheological Analysis	3
Optical Property	3-4
Thermionic emission theory	4
References	5

### Rheological Analysis:

The strain-sweep experiment, performed at a constant angular frequency of 6.283 rad/s, provided insights into the gel's mechanical response under varying strain conditions. The results, depicted in Fig. S1, highlight the Cu-IPA metallogel's ability to maintain its structure and mechanical integrity within specific strain limits, further emphasizing its high tolerance and gel stability.



**Fig. S1.** Strain-sweep measurements of Cu-IPA metallogel performed at a constant frequency of 6.283 rad/sec.

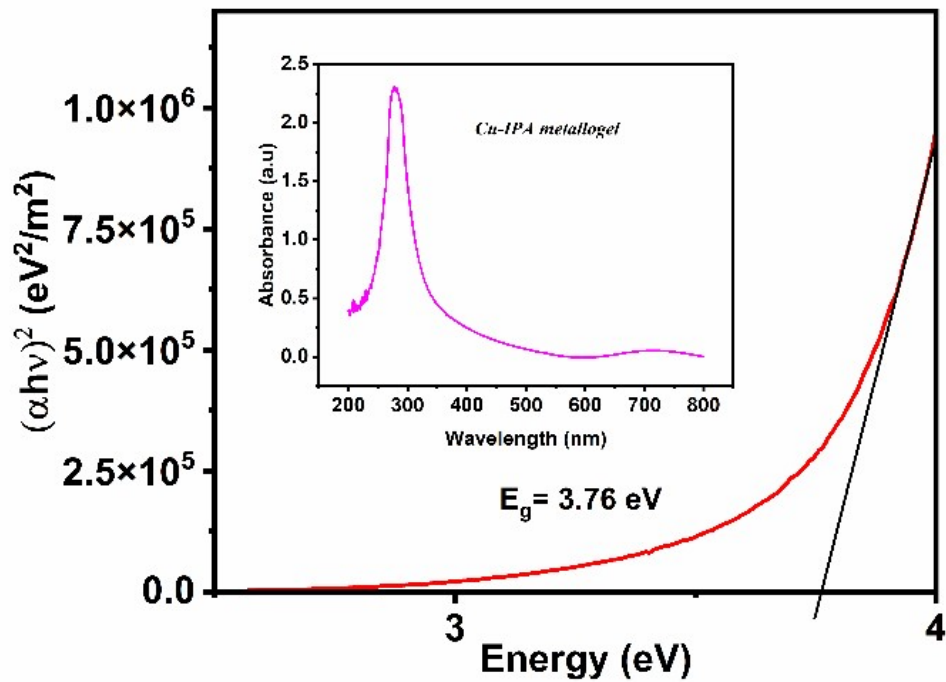
### Optical Property:

In order to ascertain the optical band gap, the optical absorbance spectra of the synthesized metallogel were measured. The UV-Vis absorption spectrum of the synthesized material between 200 and 800 nano-meters is shown in Fig. S2 inset. The metallogel's direct optical band gap energy is determined using Tauc's equation<sup>1</sup>

$$(\alpha h\nu)^2 = c(h\nu - E_g) \quad (S1)$$

where  $\alpha$  is the absorption coefficient,  $E_g$  is the optical band gap energy,  $h$  is Planck's constant,  $\nu$  is frequency and  $c$  refer a constant. The band gap energy due to direct allowed

transitions in the metallogel is estimated as 3.76 eV (Fig. S2) considering highest absorption edge in Tauc's plot.



**Fig. S2.** Tauc's plot to evaluate the direct allowed band gap energy and (inset) UV-Vis absorption spectra of the metallogel.

### Thermionic emission theory:

For the very purpose the following equations of thermionic emission is employed where series resistance of the configuration is also taken into consideration.<sup>2</sup>

$$I = I_{sat} \left( e^{\frac{q(V - IR_s)}{nkT}} - 1 \right) \quad (S2)$$

Where  $I_{sat}$  represents the saturation current density,  $q$  is the electronic charge,  $V$  symbolizes the voltage across the diode,  $n$  is the ideality factor,  $k$  denotes the Boltzmann constant and  $T$  is the absolute temperature.  $IR_s$  is the voltage drop across the configuration with a series resistance of  $R_s$ . The saturation current density  $I_{sat}$  can be expressed as:

$$I_{sat} = AA^*T^2 e^{\frac{-q\phi_b}{kT}} \quad (S3)$$

Where  $A^*$  is the effective Richardson constant and  $\phi_b$  is the formed barrier height between Al/Cu-IPA-metallogel interface. Here, the effective diode area is considered as  $7.065 \times 10^{-6} \text{ m}^2$ . The effective Richardson constant is taken as  $1.201 \times 10^6 \text{ AK}^{-2}\text{m}^{-2}$  using standard value of the constant.

**Reference:**

1. A. Dolgonos, T. O. Mason and K. R. Poeppelmeier, *J. Solid State Chem.*, 2016, **240**, 43-48.
2. P. Das, B. Pal, J. Datta, M. Das, S. Sil and P. P. Ray, *J. Phys. Chem. Solids*, 2021, **148**, 109706.