Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

A photonic multifunctional moleculator powered by two-step energy transfer

Provakar Paul[a], Monaj Karar[a], Arabinda Mallick[b]*, and Tapas Majumdar[a]*

[a]Department of Chemistry, University of Kalyani, Kalyani, Nadia, West Bengal, India – 741 235.

[b]Department of Chemistry, Kazi Nazrul University, Asansol, Burdwan, West Bengal, India – 713 340.

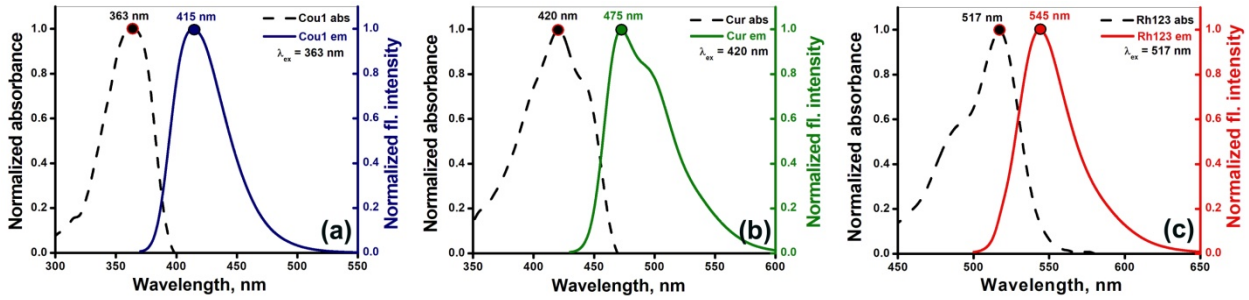

Fig. S1 Absorption (broken lines) and emission (solid lines) spectra of (a) Cou1, (b) Cur, and (c) Rh123; for absorption: [Cou1] = 4.0 μM, [Cur] = 5.2 μM, [Rh123] = 3.5 μM; for emission: [Cou1] = 0.37 μM, [Cur] = 1.99 μM, [Rh123] = 1.05 μM; solvent: DiOx; temp. = 300 K.

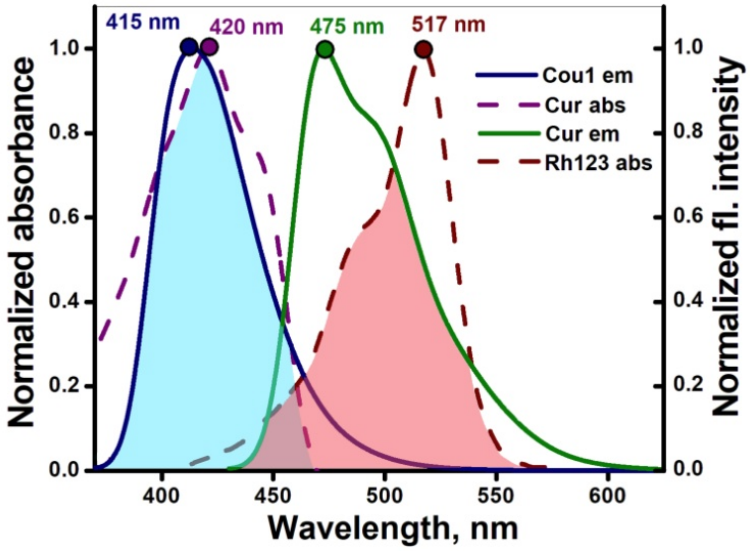

Fig. S2 Overlapping of emission-absorption spectra of two dye pairs: Cou1-Cur (sky blue) and Cur-Rh123 (light red).

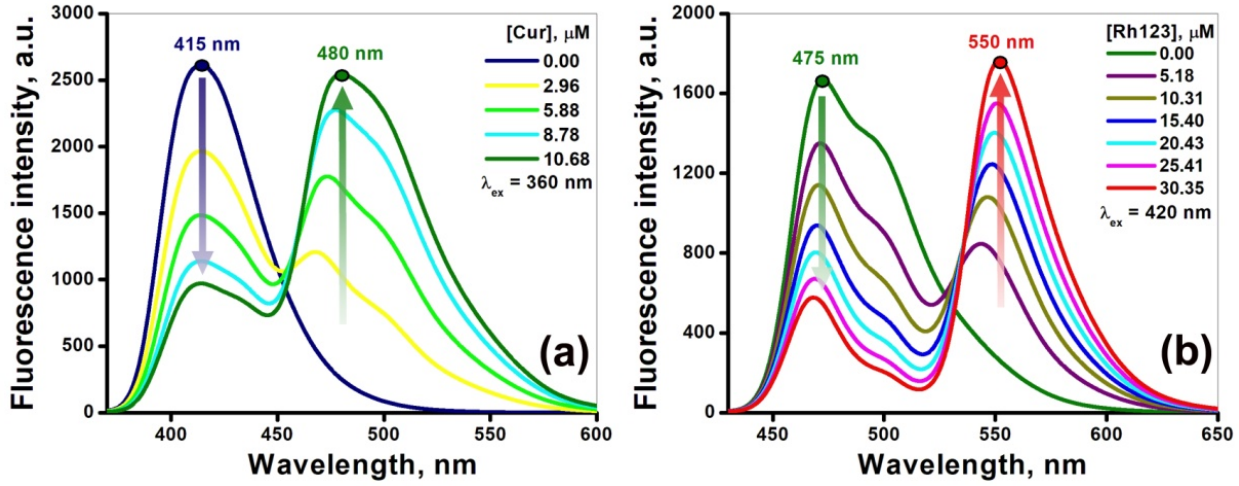

Fig. S3 Energy transfer between two individual dye pairs, (a) Cou1-Cur (Ex 360 nm, Em shift: 415 to 480 nm), [Cou1] = 0.37 μM and [Cur] = 0 to 10.68 μM; (b) Cur-Rh123 (Ex 420 nm, Em shift: 475 to 550 nm), [Cur] = 1.99 μM, [Rh123] = 0 to 30.35 μM; solvent: DiOx; temp. = 300 K.

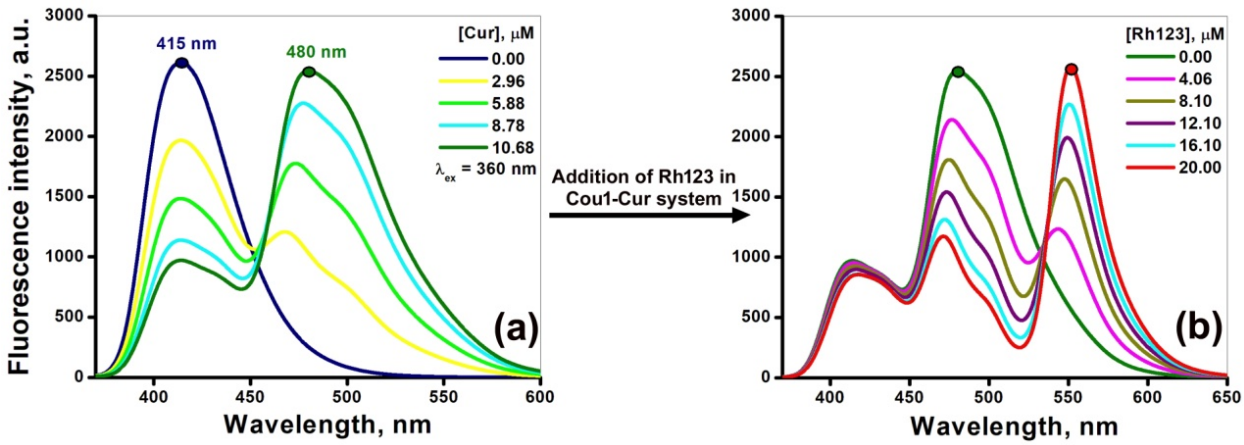

Fig. S4 (a) Changes in the emission spectra of Cou1 (0.37 μM) upon gradual addition of Cur (up to 10.68 μM); (b) changes in the emission spectra of Cou1-Cur system upon gradual addition of Rh123 (up to 20 μM); λ_{ex} = 360 nm; solvent: DiOx; temp. = 300 K.

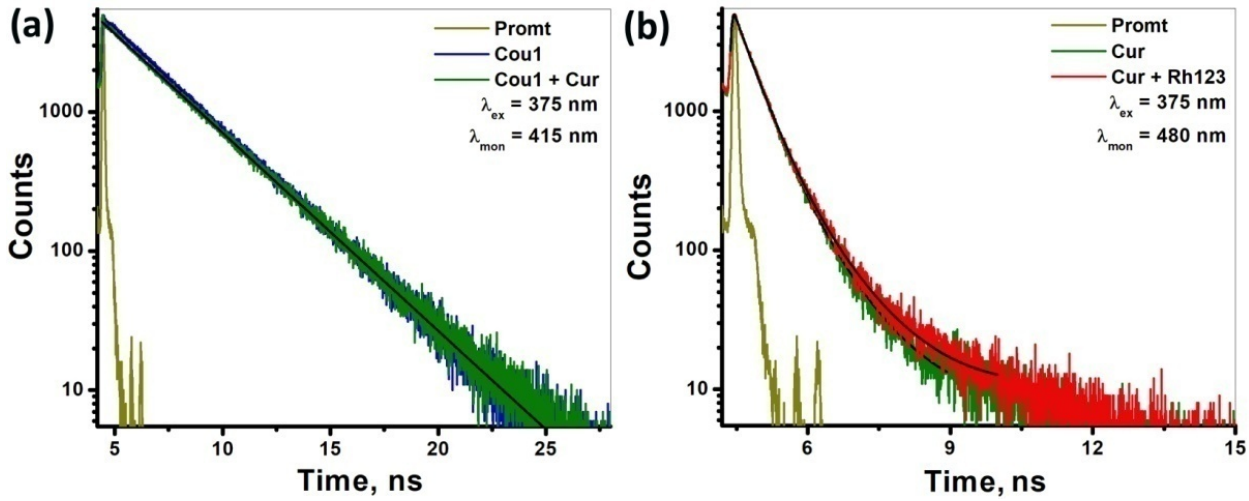

Fig. S5 Time-resolved fluorescence decay profiles of (a) Cou1 in absence and presence of Cur, λ_{ex} = 375 nm; λ_{mon} = 415 nm; (b) Cur in presence and absence of Rh123 in Cou1-Cur system, λ_{ex} = 375 nm; λ_{mon} = 480 nm; [Cou1] = 0.37 μM, [Cur] = 10.68 μM, [Rh123] = 20 μM; solvent: DiOx; temp. = 300 K.

Table S1 Time resolved decay parameters of Cou1, Cou1-Cur and Cou1-Cur-Rh123 systems excited at 375 nm and monitored at 415 and 480 nm. χ^2 represents the goodness of fitting. The data are within ±5% error limit. [Cou1] = 0.37 μM, [Cur] = 10.68 μM, [Rh123] = 20 μM; solvent: DiOx; temp. = 300 K.

Dye system	Monitoring emission wavelength				
	415 nm		480 nm		
	T_1 (ns), {α_1 (%)}	χ^2	T_1 (ns), {α_1 (%)}	T_2 (ns), {α_2 (%)}	χ^2
Cou1	2.99, {100}	1.15	-	-	-
Cou1-Cur	3.04, {100}	1.17	0.42, {77.87}	0.95, {22.13}	1.16
Cou1-Cur-Rh123			0.41, {73.35}	0.95, {26.65}	1.04

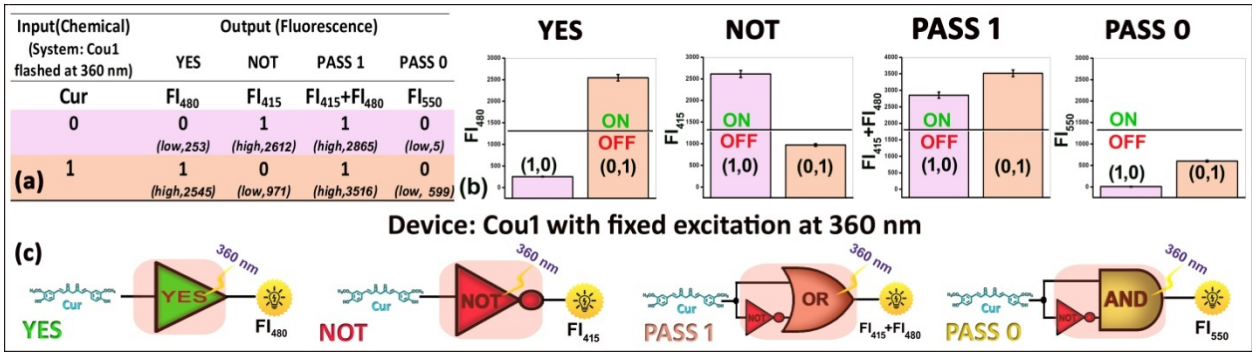

Fig. S6 (a) Truth tables, (b) bar diagrams, and (c) presentation of single-input-single-output logic gates based on two-step energy transfer; [Cou1] = 0.37 μM, [Cur] = 10.68 μM; solvent: DiOx; temp. = 300 K.

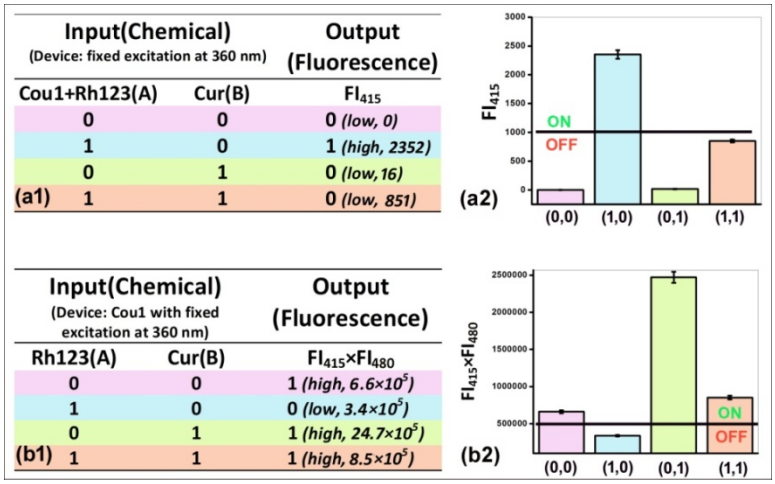

Fig. S7 Truth tables and bar diagrams for the (a) REVERSE INHIBIT, and (b) REVERSE IMPLICATION logic gates based on two-step energy transfer; [Cou1] = 0.37 μM, [Cur] = 10.68 μM, [Rh123] = 20 μM; solvent: DiOx; temp. = 300 K.

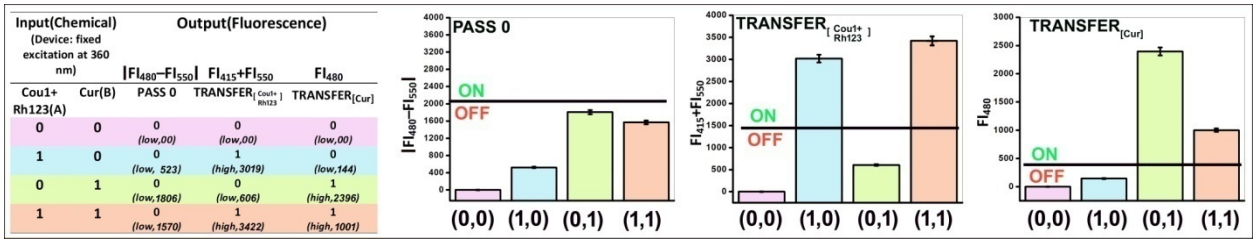

Fig. S8 Truth tables and bar diagrams for the dual-input PASS 0, TRANSFER$_{[Cou1+Rh123]}$ and TRANSFER$_{[Cur]}$ logic gates based on two-step energy transfer; [Cou1] = 0.37 μM, [Cur] = 10.68 μM, [Rh123] = 20 μM; solvent: DiOx; temp. = 300 K.

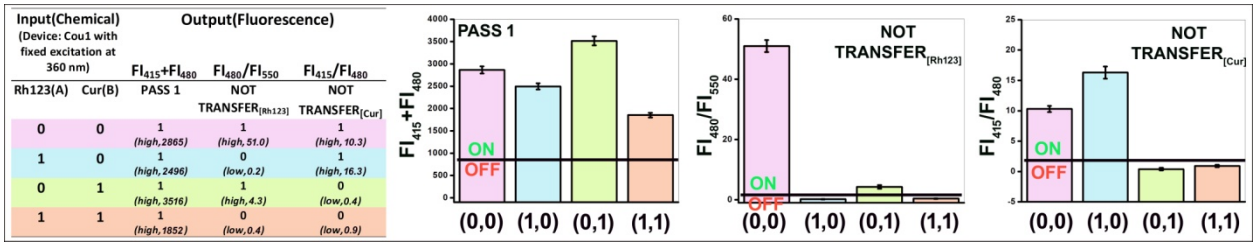

Fig. S9 Truth tables and bar diagrams for the dual-input PASS 1, NOT TRANSFER$_{[Rh123]}$ and NOT TRANSFER$_{[Cur]}$ logic gates based on two-step energy transfer; [Cou1] = 0.37 μM, [Cur] = 10.68 μM, [Rh123] = 20 μM; solvent: DiOx; temp. = 300 K.

Relative quantum yield calculation:

Relative fluorescence quantum yields (φ_f) of Cou1, Cur and Rh123 in DiOx were determined considering the fluorescence quantum yields of Cou1 in Acetonitrile ($\varphi_{\text{Cou 1}}^{\text{ACN}} = 0.62$)[S1], Cur in Isopropanol ($\varphi_{\text{Cur}}^{\text{iPrOH}} = 0.114$)[S2] and Rh123 in Ethanol ($\varphi_{\text{Rh 123}}^{\text{EtOH}} = 0.86$)[S3] as the references, respectively. The relative fluorescence quantum yields of Cou1, Cur and Rh123 were calculated by using equation S1, where, φ_x is the relative fluorescence quantum yield of sample, φ_r is the fluorescence quantum yield of the respective reference, A_x and A_r are the absorbance of sample and the reference, respectively, F_x and F_r are the area of emission for sample and the reference, respectively, n_x and n_r are the refractive indices of the sample and reference solutions. The absorbance of all the dye solutions at the excitation wavelength were kept below 0.1 and all the relative quantum yield measurements were carried out in identical experimental conditions.

$$\varphi_x = \varphi_r \times \frac{A_r}{A_x} \times \frac{F_x}{F_r} \times \frac{n_x^2}{n_r^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(eq. S1)}$$

References

S1. A. Barik, S. Nath and H. Pal, *J. Chem. Phys.*, 2003, **119**, 10202–10208.

S2. K. I. Priyadarsini, *J. Photochem. Photobiol. C*, 2009, ***10***, 81–95.

S3. P. Pal, H. Zeng, G. Durocher, D. Girard, R. Giasson, L. Blanchard, L. Gaboury and L. Villeneuve, *J. Photochem. Photobiol. A*, 1996, **98**, 65-72.