*Supplementary Information*

# 1D Cu(I)-based chiral organic-inorganic hybrid material with second harmonic generation and circular polarized luminescence

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**Supporting Figures:**

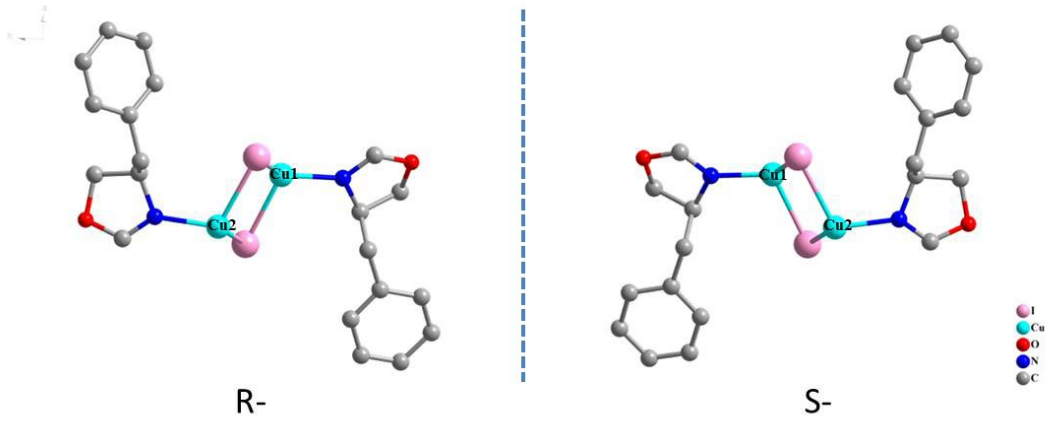
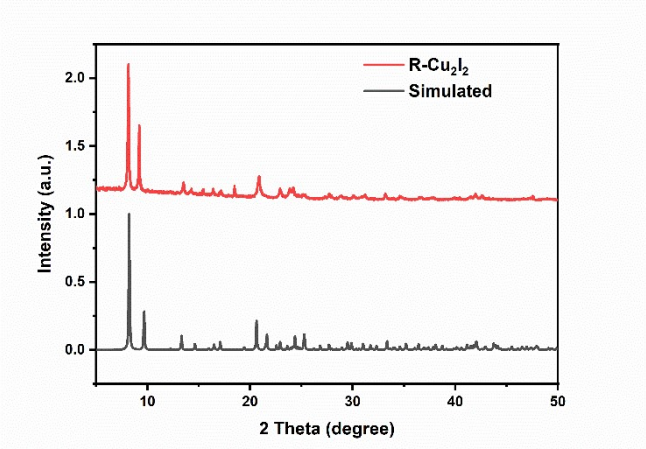
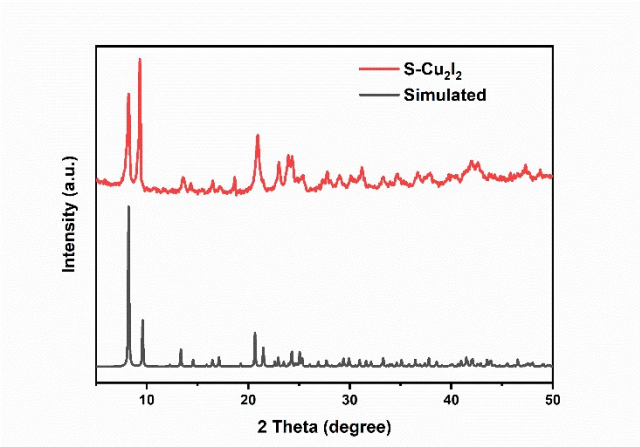



**Fig. S1.** The asymmetric units of the *R*/*S*- $Cu_2I_2$.

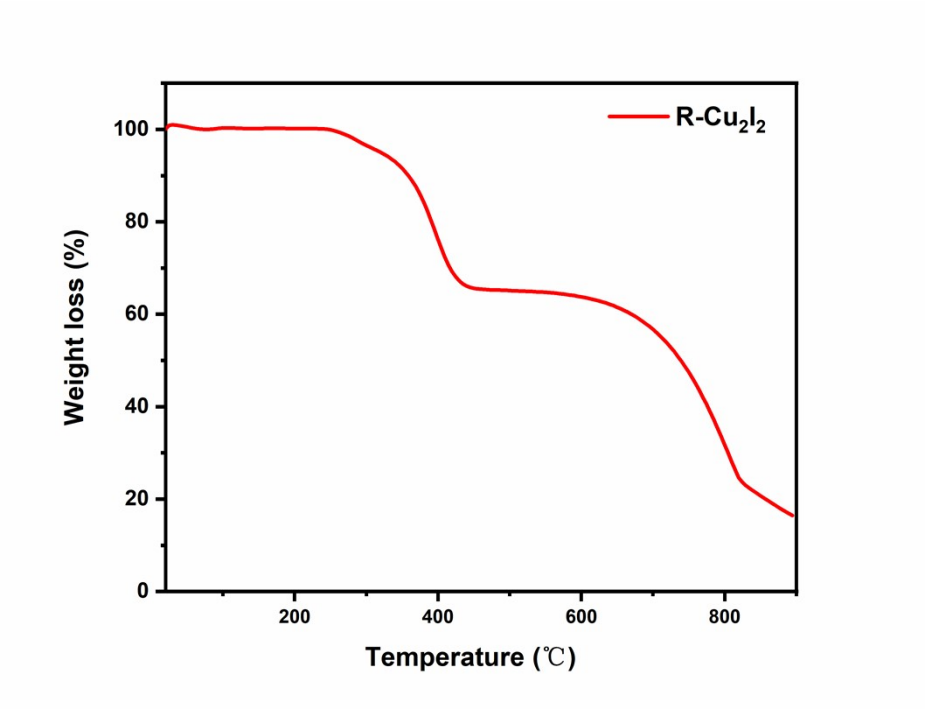



**(a)**

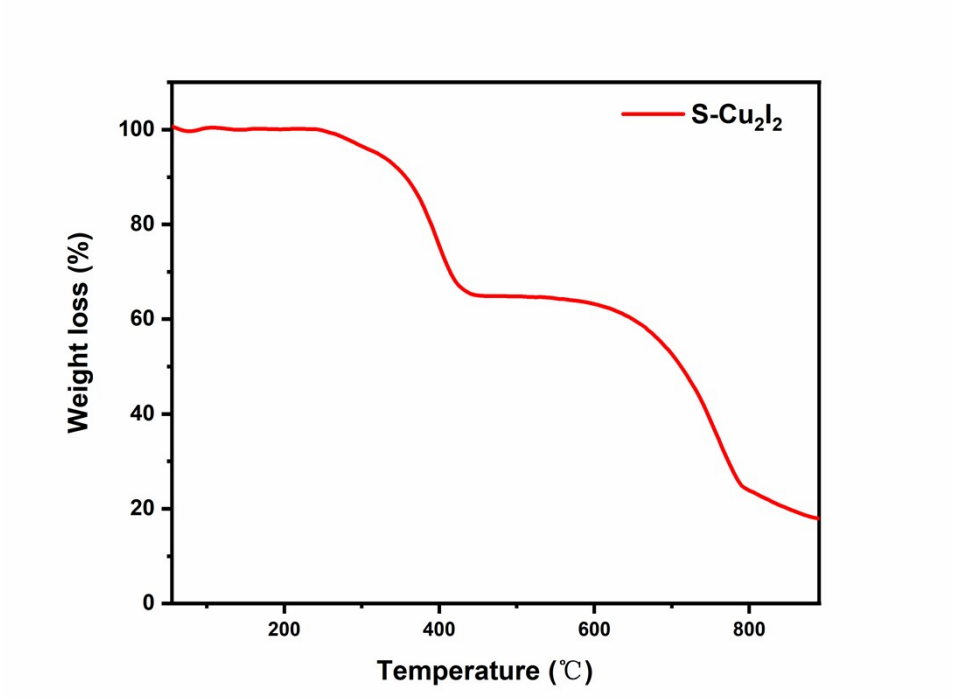



**(b)**

**Fig. S2.** Simulated and experimental power XRD patterns of *R*-$Cu_2I_2$ (a) and *S*-$Cu_2I_2$ (b).

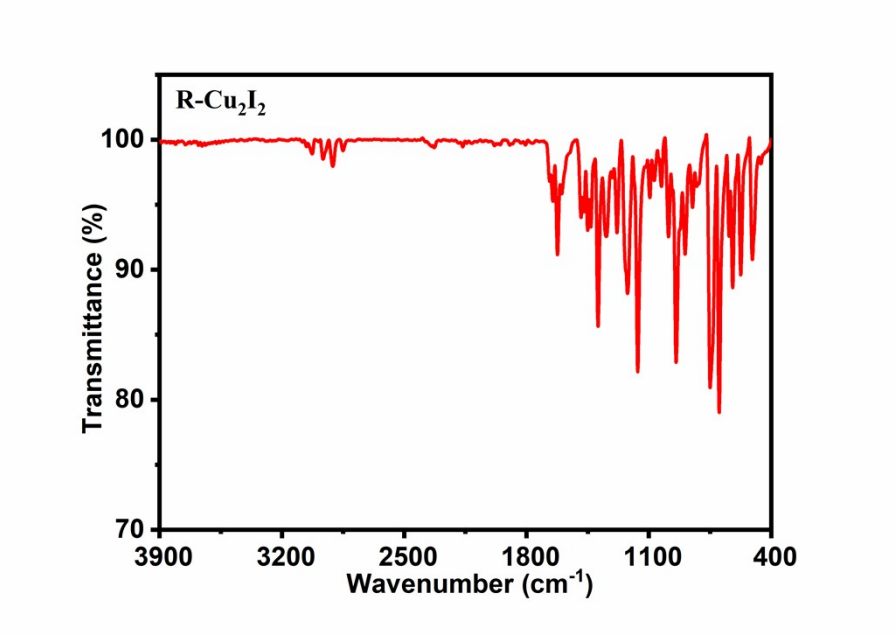



(a)

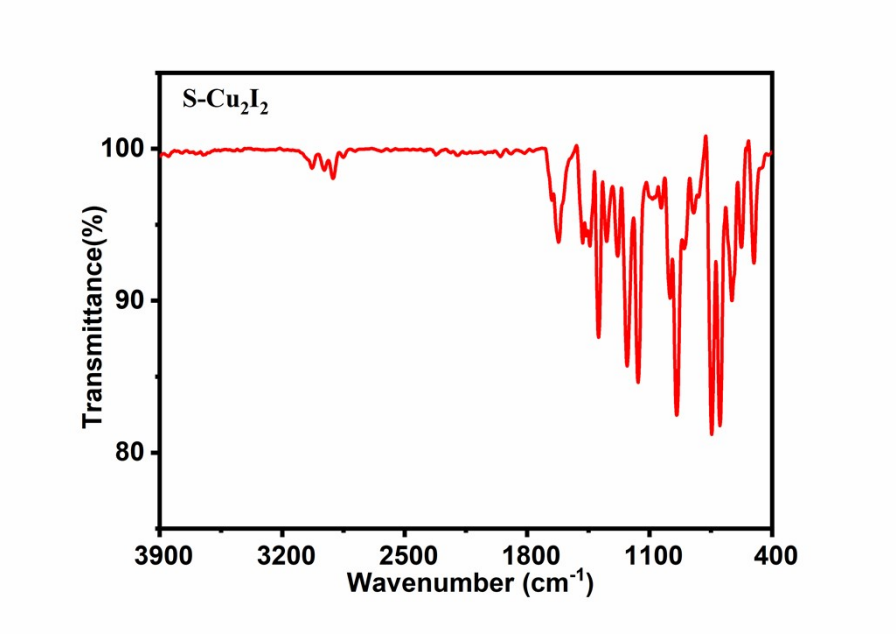



(b)

**Fig. S3.** The TGA curves of *R*-$Cu_2I_2$ (a) and *S*-$Cu_2I_2$ (b).




(a)




(b)

**Fig. S4.** Infrared spectra of *R*-$Cu_2I_2$ (a) and *S*-$Cu_2I_2$ (b).

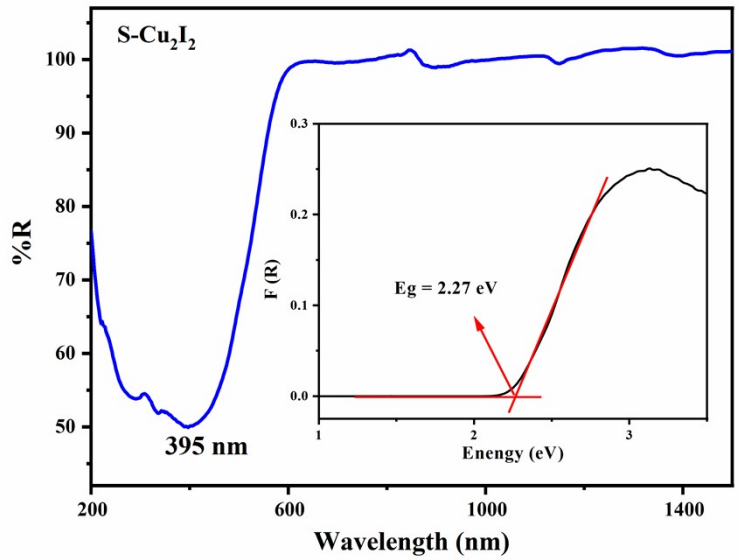



**Fig. S5.** UV-vis diffuse reflectance spectrum and experimental bandgap for *S*-$Cu_2I_2$.

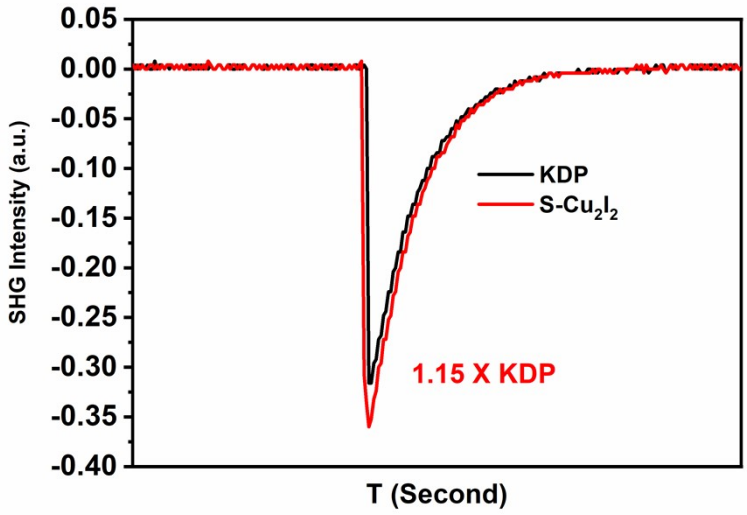
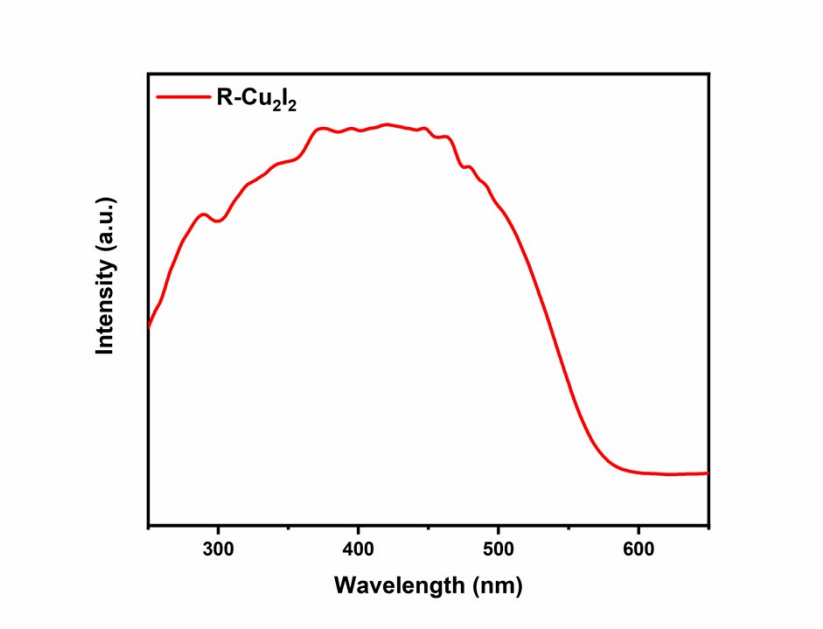
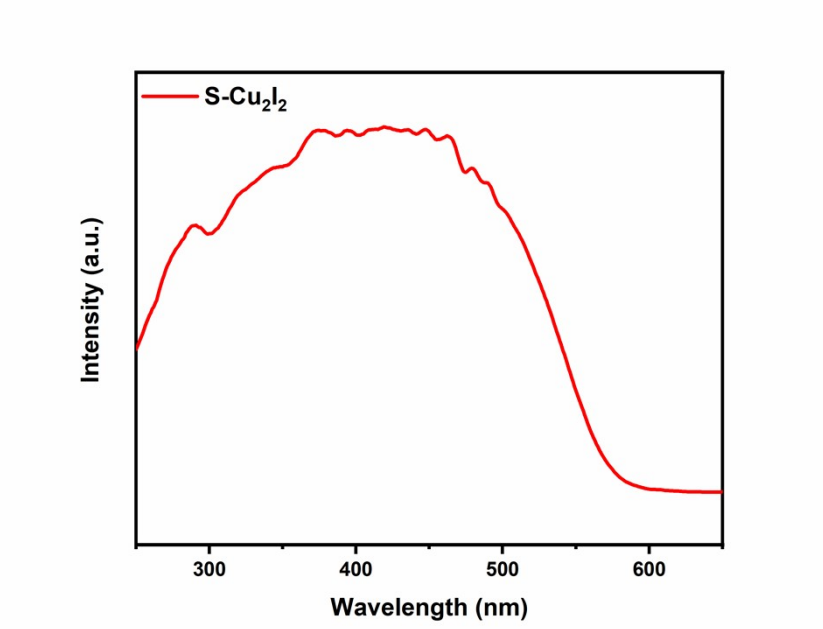



**Fig. S6.** Comparison of SHG intensities between *S*-$Cu_2I_2$ and KDP.




(a)




(b)

**Fig. S7.** Excitation spectra of *R*-$Cu_2I_2$ (a) and *S*-$Cu_2I_2$ (b).

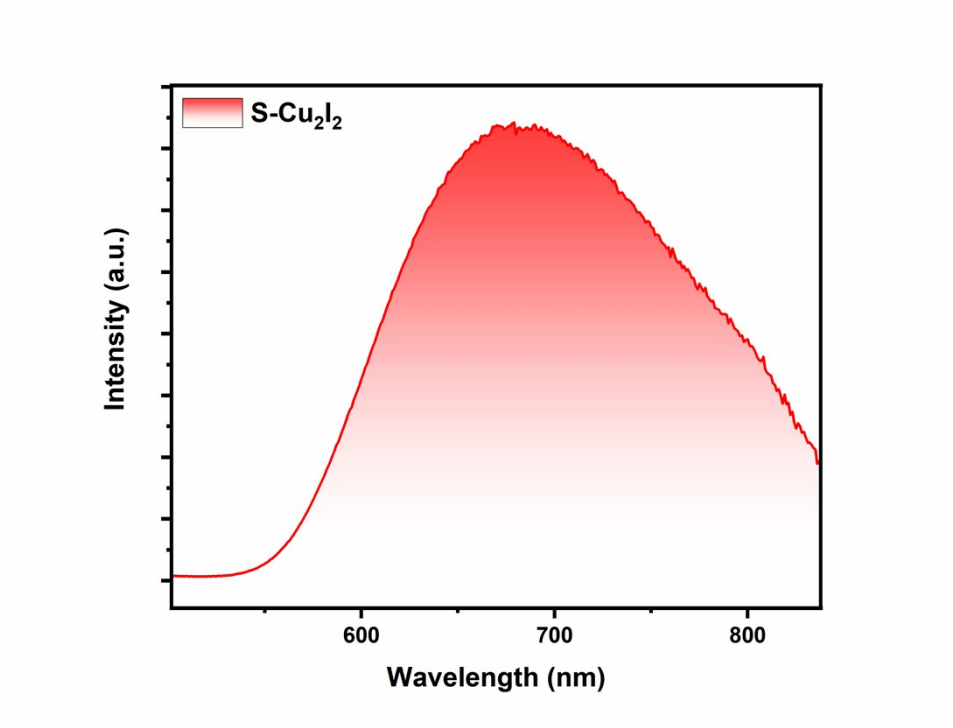



**Fig. S8.** Emission spectrum of *S*-$Cu_2I_2$.

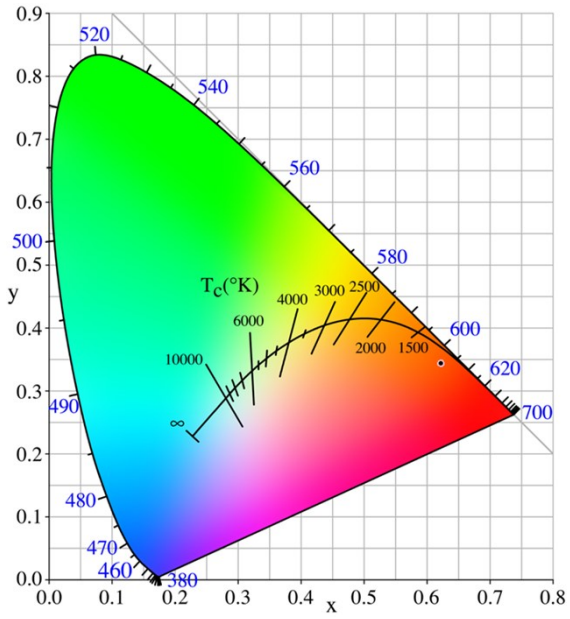
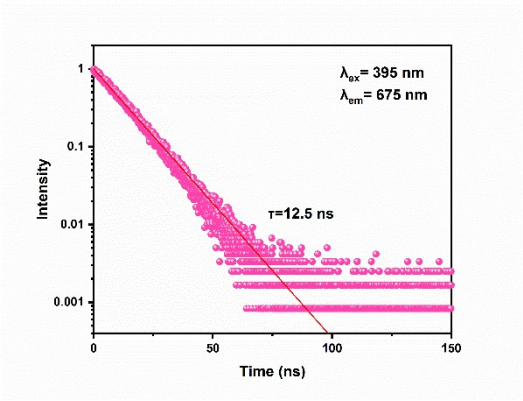
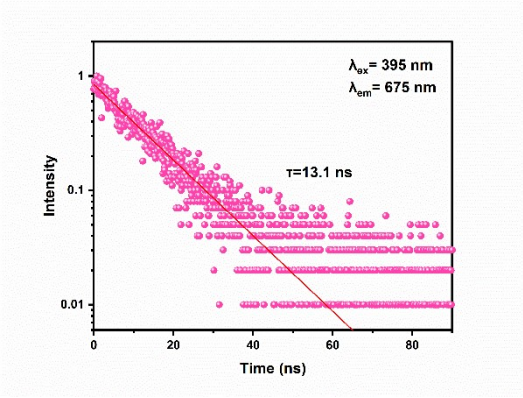



**Fig. S9.** The chromaticity coordinate diagram of *S*-$Cu_2I_2$.




**(a)**




**(b)**

**Fig. S10.** Time-resolved PL decay curves of *R*-$Cu_2I_2$ (a) and *S*-$Cu_2I_2$ (b).

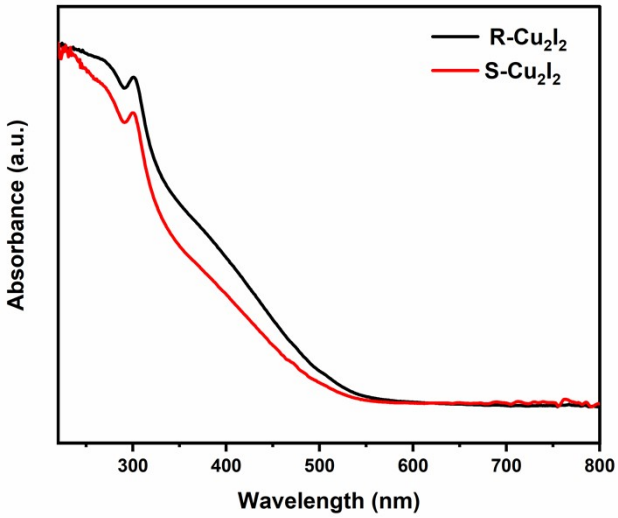



**Fig. S11.** Ultraviolet absorption spectra of *R*/S-$Cu_2I_2$.

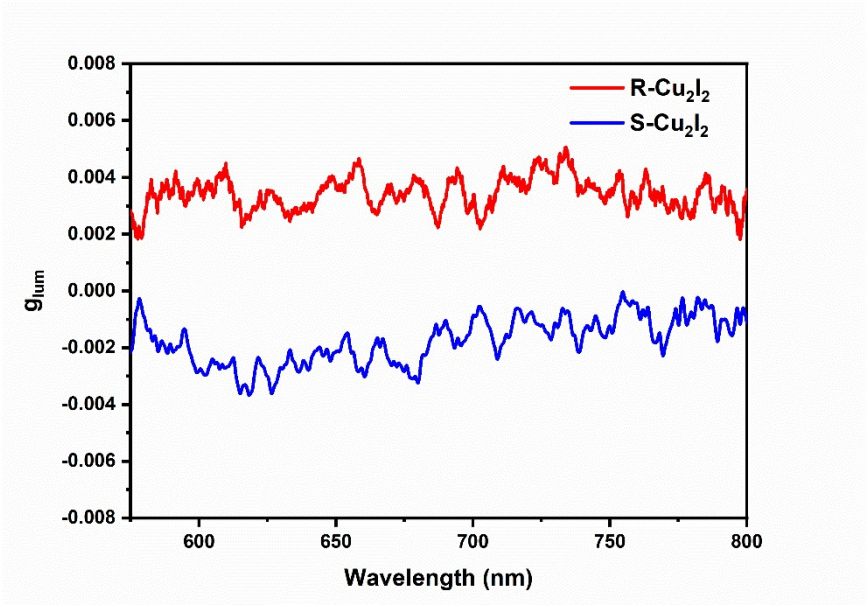



**Fig. S12.** Asymmetry factor $g_{lum}$ curves of *R*/*S*-$Cu_2I_2$.

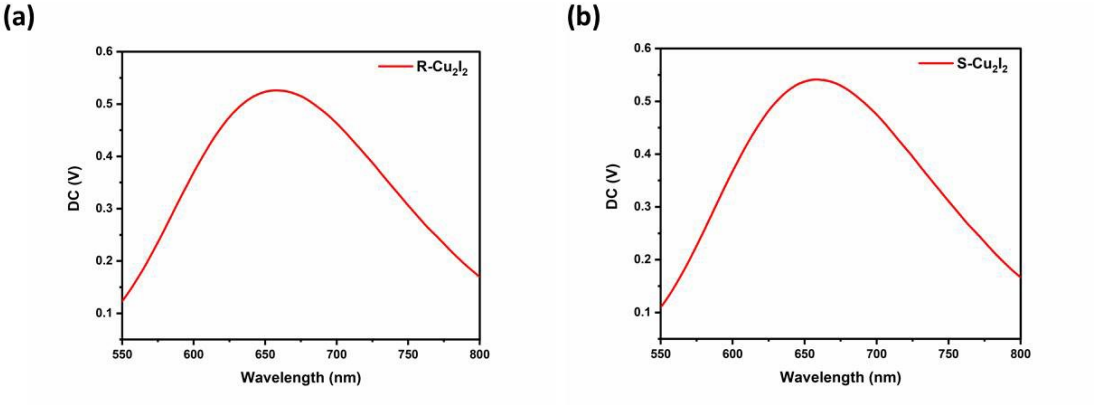



**Fig. S13.** DC spectra of *R*/*S*-$Cu_2I_2$.

**Supporting Table:**

Table S1. Crystal data and structure refinement for *R*-$Cu_2I_2$ and *S*-$Cu_2I_2$.

| Compound | *R*-$Cu_2I_2$ | *S*-$Cu_2I_2$ |
|---|---|---|
| Crystal Formula | *R*-$C_{20}H_{20}Cu_2I_2N_2O_2$ | *S*-$C_{20}H_{20}Cu_2I_2N_2O_2$ |
| Formula weight | 701.26 | 701.26 |
| Space group | *I*2 | *I*2 |
| Crystal system | Monoclinic | Monoclinic |
| a/Å | 8.6981(2) | 8.68790(10) |
| b/Å | 13.2756(4) | 13.24430(10) |
| c/Å | 18.4773(4) | 18.54630(10) |
| α /° | 90 | 90 |
| β /° | 98.763(2) | 98.7650(10) |
| γ /° | 90 | 90 |
| V/Å$^3$ | 2108.71(9) | 2109.11(3) |
| Z | 4 | 4 |
| ρ /g cm$^{-3}$ | 2.209 | 2.208 |
| μ /mm$^{-1}$ | 25.628 | 25.623 |
| F(000) | 1336.0 | 1336.0 |
| GOF on $F_2$ | 1.007 | 1.064 |
| $R_1$[a]/$wR_2$[b] [I > 2(I)] | 0.0235/ 0.0600 | 0.0207/0.0562 |
| $R_1$[a]/$wR_2$[b] (all data) | 0.0248/ 0.0605 | 0.0210/0.0564 |
| Flack parameter | 0.001(8) | -0.016(3) |

[a]$R_1 = \Sigma||F_0| - |F_c||/\Sigma|F_0|$. [b]$wR_2 = \{\Sigma[w(F_0^2 - F_c^2)_2]/\Sigma[w(F_0^2)_2]\}^{1/2}$.

Table S2. Selected bond lengths (Å) in *R*-$Cu_2I_2$.

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| **I1** | Cu1 | 2.5813(13) | C2 | C3 | 1.530(11) |
| **I1** | Cu1[1] | 2.8113(14) | C2 | C4 | 1.522(10) |
| **I1** | Cu2 | 2.6923(13) | C4 | C5 | 1.527(10) |
| **I2** | Cu1 | 2.6659(13) | C5 | C6 | 1.390(12) |
| **I2** | Cu2 | 2.6562(13) | C5 | C10 | 1.388(11) |
| **I2** | Cu2[2] | 2.6785(12) | C6 | C7 | 1.402(11) |
| **Cu1** | Cu1[1] | 2.687(2) | C7 | C8 | 1.389(13) |
| **Cu1** | Cu2 | 2.9810(14) | C8 | C9 | 1.371(11) |
| **Cu1** | N1 | 2.014(8) | C9 | C10 | 1.403(10) |
| **Cu2** | Cu2[2] | 2.689(2) | C11 | C11[1] | 1.464(16) |
| **Cu2** | N2 | 2.043(8) | C12 | C13 | 1.512(11) |
| **O1** | C11 | 1.349(10) | C13 | C14 | 1.532(10) |
| **O1** | C12 | 1.469(9) | C14 | C15 | 1.510(10) |
| **O2** | C1 | 1.326(10) | C15 | C16 | 1.360(13) |
| **O2** | C3 | 1.470(8) | C15 | C20 | 1.388(12) |
| **N1** | C11 | 1.285(11) | C16 | C17 | 1.393(12) |
| **N1** | C13 | 1.497(9) | C17 | C18 | 1.337(14) |
| **N2** | C1 | 1.280(11) | C18 | C19 | 1.385(14) |
| **N2** | C2 | 1.497(9) | C19 | C20 | 1.402(11) |
| **C1** | C1[2] | 1.497(15) | | | |

**[1]1-X,+Y,1-Z; [2]2-X,+Y,1-Z**

Table S3. Selected bond lengths (Å) in *S*-$Cu_2I_2$.

| Atom | Atom | Length/Å | Atom | Atom | Length/Å |
|---|---|---|---|---|---|
| **I2** | Cu1 | 2.6565(7) | O1 | C2 | 1.472(5) |
| **I2** | Cu11 | 2.6757(7) | N1 | C3 | 1.501(5) |
| **I2** | Cu2 | 2.6656(7) | C10 | C9 | 1.402(6) |
| **I1** | Cu1 | 2.6918(7) | C10 | C5 | 1.396(7) |
| **I1** | Cu2 | 2.5825(7) | C9 | C8 | 1.392(7) |
| **I1** | Cu22 | 2.8076(8) | C8 | C7 | 1.373(7) |
| **Cu1** | Cu11 | 2.6882(12) | C18 | C19 | 1.368(9) |
| **Cu1** | Cu2 | 2.9765(9) | C18 | C17 | 1.379(8) |
| **Cu1** | N1 | 2.044(5) | C11 | C112 | 1.476(8) |
| **Cu2** | Cu22 | 2.6881(12) | C5 | C6 | 1.390(6) |
| **Cu2** | N2 | 2.023(5) | C5 | C4 | 1.519(5) |
| **N2** | C11 | 1.273(6) | C7 | C6 | 1.395(6) |
| **N2** | C13 | 1.496(5) | C17 | C16 | 1.392(7) |
| **C1** | C11 | 1.481(7) | C13 | C14 | 1.536(6) |
| **C1** | O1 | 1.344(6) | C13 | C12 | 1.516(7) |
| **C1** | N1 | 1.277(6) | C3 | C2 | 1.529(7) |
| **O2** | C11 | 1.344(6) | C3 | C4 | 1.519(6) |
| **O2** | C12 | 1.480(5) | C16 | C15 | 1.397(7) |
| **C20** | C19 | 1.388(7) | C15 | C14 | 1.506(5) |
| **[1]1-X,+Y,1-Z; [2]2-X,+Y,1-Z** | | | | | |