Electronic supplementary information

Construction of a viologen-derived 2D material with photochromism, photoswitchable luminescence and inkless and erasable prints *via* sunlight irradiation

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Table S1 Crystal data and structure refinements for 1.					
Compound	1				
Formula	$C_{23}H_{14}N_2O_6SZn$				
$M_{ m r}$	511.79				
Crystal system	Monoclinic				
Space group	$P2_{1}/n$				
<i>a</i> (Å)	10.146(2)				
<i>b</i> (Å)	13.915(2)				
<i>c</i> (Å)	14.641(12)				
а	90				
β (°)	96.29(7)				
γ	90				
$V(Å^3)$	2054.5(19)				
Z	4				
$\rho(\text{g cm}^{-3})$	1.655				
µ/mm ⁻¹	1.343				
<i>F</i> (000)	1040				
$GOF(F^2)$	1.068				
$R_1[I>2\sigma(I)]$	0.0360				
$wR_2[I>2\sigma(I)]$	0.0757				

Section 1. Additional Data and Figures

Table S2 Selected bond lengths (Å) and bond angles (°) for 1.

Compound 1 ^a							
Zn(1)-O(1)	1.9037(16)	Zn(1)-O(4)#1	2.0191(17)	Zn(1)-O(5)	1.961(2)		
Zn(1)-N(2)#2	2.124(2)						
O(5) - Zn(1)- O(4)#1	94.75(8)	N(2)#2-Zn(1)-O(1)	125.29(8)	O(1)-Zn(1)-O(5)	108.74(8)		
O(5)-Zn(1)-N(2)#2	103.87(9)	O(4)#1-Zn(1)-N(2) #2	109.60(8)	O(4)#1-Zn(1)-O(1)	110.04(7)		
^a Symmetry codes: #1 5/2-X,1/2+Y,1/2-Z; #2 1/2-X,1/2+Y,1/2-Z.							



Fig.S1 PXRD patterns for 1.



Fig.S2 TGA curve for 1.



Fig.S3 The kinetic rate constant of compound 1 for sunlight conversion based on 602 nm.



Fig. S4. PXRD patterns of compound 1 and 1 after irradiation.



Fig. S5 detail of the structure of compound 1 showing short contacts involving the bipyridinium unit.



Fig. S6 detail of the structure of 1 before and after light irradiation.



Fig. S7 The photoluminescence spectra of free H_2L upon excitation at 278 nm and cpbpy upon excitation at 373 nm.

Section 2. Calculation details

1) Kinetic rate calculation

After sunlight irradiation for 10 s, 20 s, 30 s, 40 s and 60 s. The UV–vis absorption spectroscopy were recorded and the calculation of kinetics of photoreaction kinetic rates was based on the intensity values of the wavelength at 602 nm. The kinetic rate constants are determined by the following equation is used for data treatment:

$$ln \frac{A_{\infty} - A_0}{A_{\infty} - A_t} = kt$$

where k is the first-order rate constant and A_0 , A_t , A_{∞} refer to the observed absorption data at 602 nm at the beginning, versus time, and at the end of the reaction, respectively.

2) DOS calculation details

We have employed the CASTEP module [S1] of the Materials Studio package to perform all density functional theory (DFT) calculations within the generalized gradient approximation (GGA) using the Perdew-Burke-Ernzerhof (PBE) [S2] formulation. We have chosen the projected augmented wave (PAW) potentials [S3,S4] to describe the ionic cores and take valence electrons into account using a plane wave basis set with a kinetic energy cutoff of 500 eV. $3 \times 2 \times 2$ k-points sampling was used for structure optimization. The electronic energy was considered self-consistent when the energy change was smaller than 10^{-5} eV. A geometry optimization was considered convergent when the energy change was smaller than 0.03 eV Å⁻¹.

References

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