Highly stable photochromic crystalline material based on a close-packed layered metal-viologen coordination polymer

Yi Tan, Zhiyong Fu, Yu Zeng, Hengjun Chen, Shijun Liao, Jie Zhang and Jingcao Dai

Experimental Section

All the reagents were purchased from commercial channels and used without further purification; N-(3-carboxyphenyl)-4,4΄-bipyridinium chloride was synthesized as reported. UV-Visible spectral measurements were carried out using a HITACHI U-3010 spectrometer (crystalline sample in a solid sample holder). A TA Instrument Q600 SDT thermogravimetric analyzer was used to obtain the TGA curve in N₂ at a rate of 10ºC min⁻¹. The ESR spectra were recorded at room temperature with a Bruker EMX-10/12 Electron Spin Resonance Spectrometer. IR spectra were characterized by a Bruker Tensor 27 FTIR spectrometer in the range of 4000-400 cm⁻¹ using a KBr disk.

A solution of Cd(NO₃)₂·4H₂O(0.2mmol, 61.7mg), m-H₂BDC (0.2mmol, 33.2mg), N-(3-carboxyphenyl)-4,4΄-bipyridinium chloride (0.1mmol, 31mg), DMF(5ml), H₂O(5ml) was stirred for 10min. The mixture was sealed in a 23ml Teflon-lined steel bomb and heated at 120ºC for 1440min. Yellow block-like crystals were collected by filtration, washed by water and ethanol, and dried at room temperature (0.06mmol, 34mg, 60% yield based on N-(3-carboxyphenyl)-4,4΄-bipyridinium chloride).
The calculation of kinetic rate constants:

After irradiation UV-Vis spectra are recorded and the calculations of kinetics of light reversion base on the intensity values of the wavelength at 616 nm. The kinetic rate constants are determined by the literature calculation method. The following equation is used for data treatment:

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

where \( A_0 \), \( A_t \), \( A_\infty \) are the observed absorption data (616 nm) at the beginning, versus time, and at the end of the reaction, respectively.

Figure S1. Thermal gravimetric curve of compound 1.
Figure S2. IR spectrum of 1