Supporting Information

An uncommon 3-D topological net based on weak metallophilic (Cu···Cu) interactions

Jian Zhou, Xiaofeng Tan, Feilong Hu, Hua-Hong Zou, Lianshe Fu, and Rongqing Zhao

General Remarks. All analytical grade chemicals were obtained commercially and used without further purification. IR spectra were obtained from a powdered sample pelletized with KBr on an ABB Bomen MB 102 series IR spectrophotometer in the range of 400–4000cm^{-1}. Room-temperature optical diffuse reflectance spectra of the powdered samples were obtained with a Shimadzu UV-3150 spectrometer. The absorption data were calculated from reflectance spectra by using the Kubelka–Munk function: a/S = (1-R^2)/2R, where a is the absorption coefficient, S is the scattering coefficient, and R is the reflectance. Fluorescence spectral analyses were performed using a Cary Eclips fluorescence spectrometer. PXRD patterns were obtained using a Bruker D8 Advance XRD diffractometer with Cu Kα radiation (λ = 1.54056 Å).

Computational descriptions. The density of states (DOS) of **1** was theoretically calculated by using the computer code CASTEP. The total energy is calculated with the density functional theory (DFT) using the Perdew–Burke–Ernzerh of generalized gradient approximation (GGA) [J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett*., 1996, **77**, 3865]. The following orbital electrons are treated as valence electrons: H 1s^1, N 2s^{2}2p^3, C 2s^{2}2p^2, O 2s^{2}2p^4 and Cu 3d^{10}4s^1. The number of plane waves included in the basis is determined by a cutoff energy of 340 eV, and the numerical integration of the Brillouin zone is performed using a Monkhorst-Pack k point sampling: 4×4×4 for **1**. The Fermi level (E_f = 0 eV) was selected as the reference of the energy.

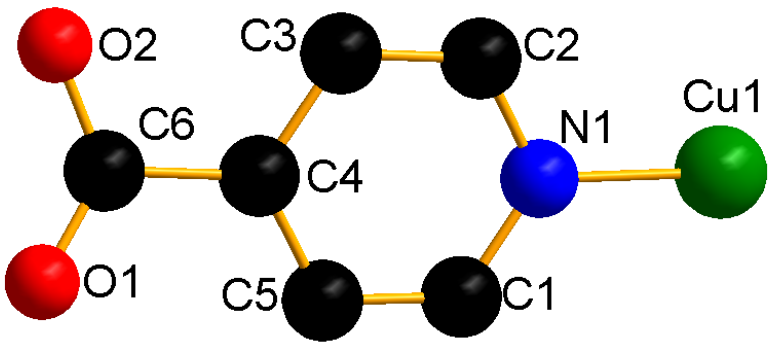
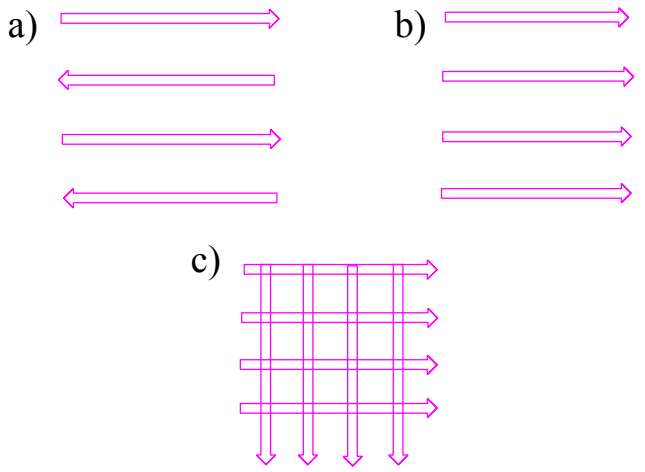


Fig. S1 The asymmetric unit of **1** (H atoms bonded to C atoms have been omitted for clarity).



Scheme S1. Stacking Modes of 1-D chains {(a) type I, (b) type II, (c) type III}.

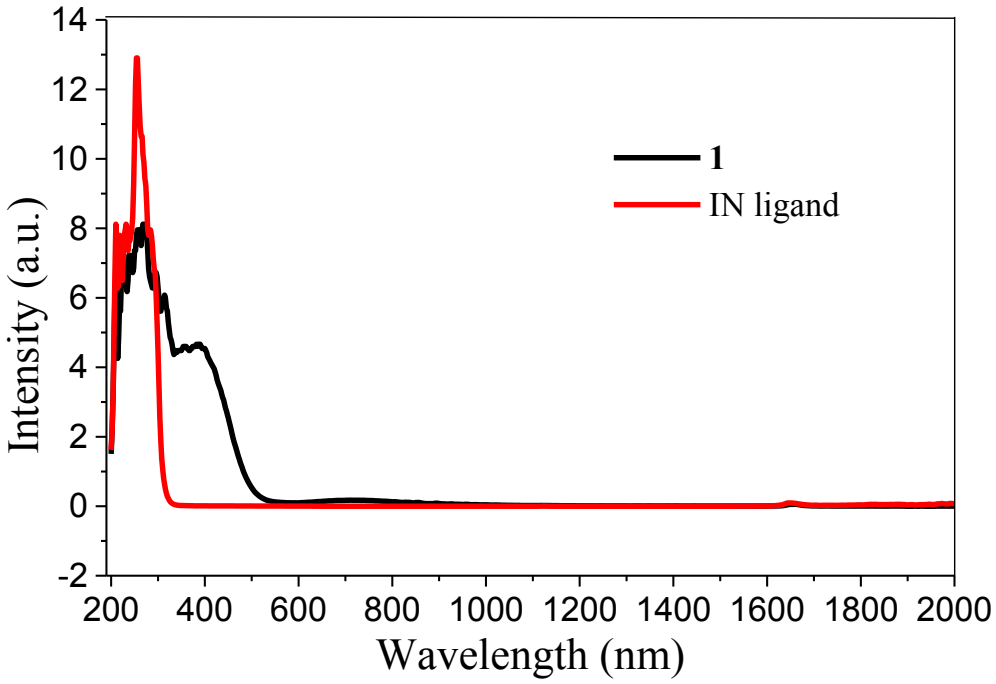


Fig. S2 UV-vis absorption spectra of the free IN ligand and **1.**

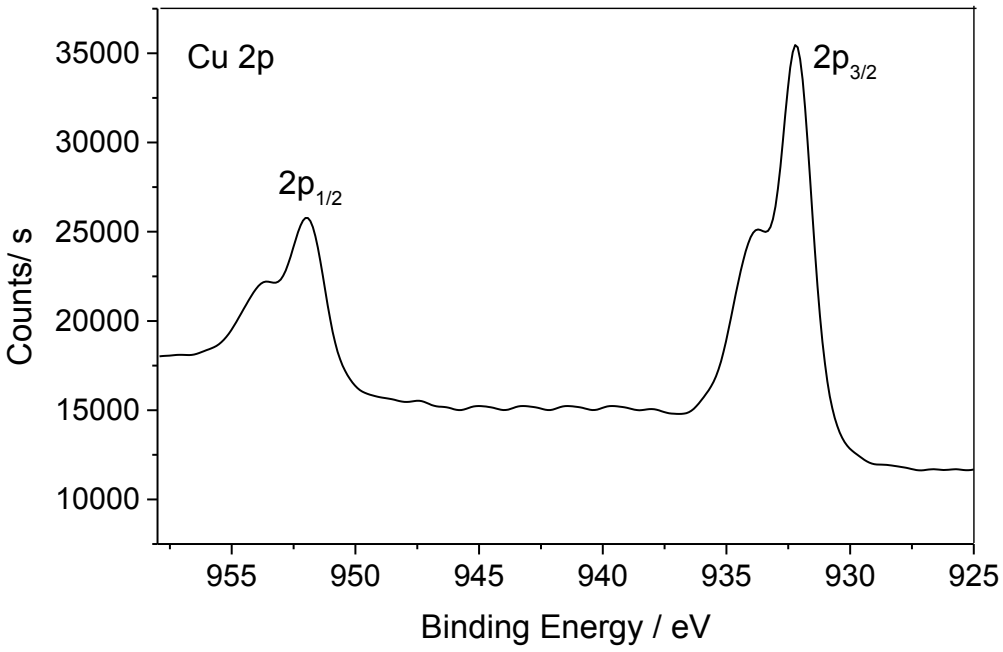


Fig. S3 Cu 2p XPS spectrum of **1.**

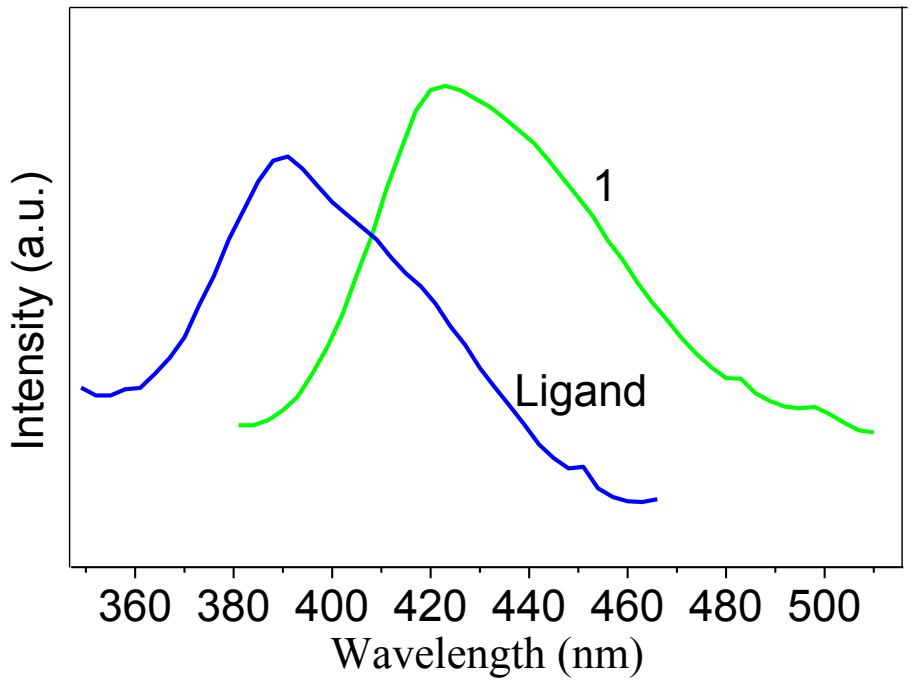


Fig. S4 The solid-state photoluminescent spectra of **1** and ligand at room temperature.

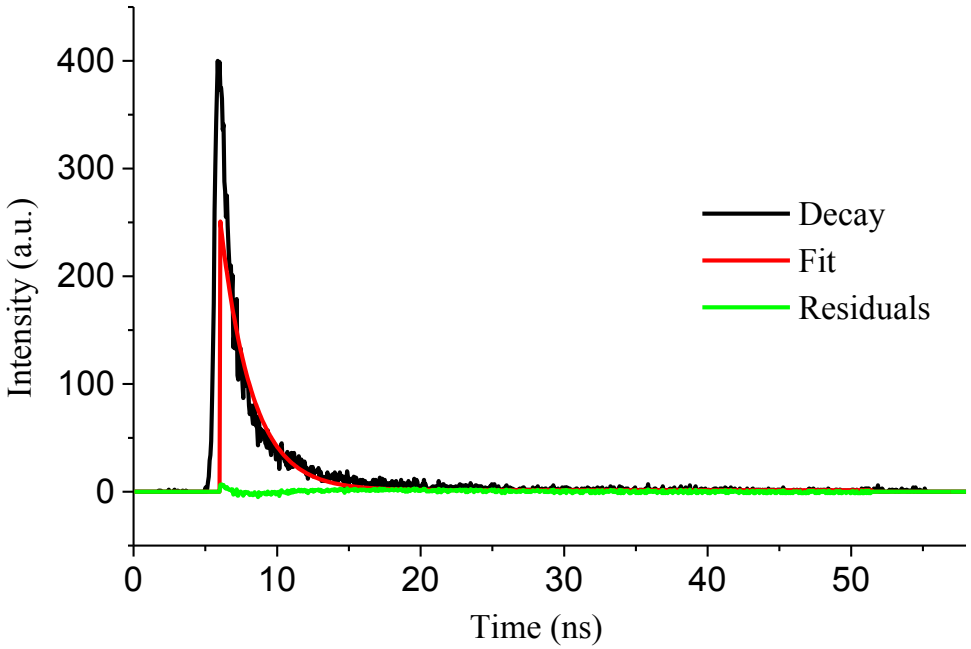


Fig. S5 Decay life time curve of **1**.

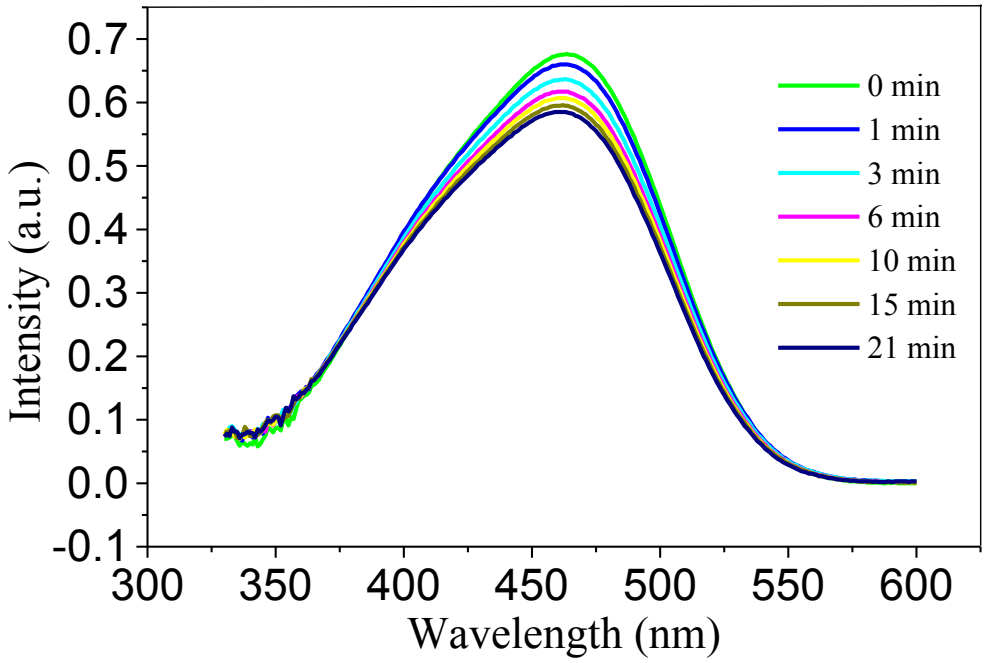


Fig. S6 UV-vis absorption spectra for degradation of methyl orange by using **1** as photocatalyst.

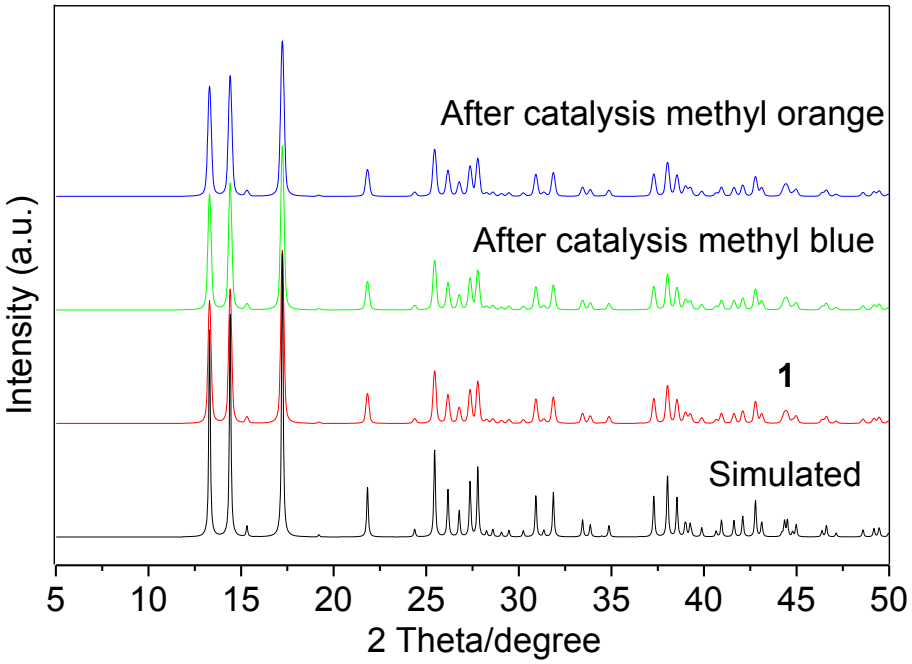


Fig. S7 Simulated, experimental and after catalysis of methyl blue or methyl orange powder XRD patterns of **1**.