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 400–4000 cm\(^{-1}\). 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 Ka radiation (\(\lambda = 1.54056\) 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: \(4\times4\times4\) 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).](image-url)
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.