

Supporting Information for

**Discrete Supertetrahedral CuInS Clusters and Its Application in
Fabrication of Cluster-Sensitized TiO₂ Photoelectrodes**

Zhao-Qi Li, Chong-Jiao Mo, Yao Guo, Nan-Nan Xu, Qin-Yu Zhu,* and Jie Dai*

College of Chemistry, Chemical Engineering and Materials Science, Soochow
University, Suzhou 215123, P. R. China

Table S1. Crystal data and structural refinement parameters for **1**.

Table S2. Solubility of compound **1** in different solvents with LiBr.

Figure S1. XPS spectra of **1**, showing the Cu2p peaks, which are in agreement with that of Cu(I).

Figure S2. Absorption spectra of **1** in DMF with 0.2 mol/L LiBr. Insert is the picture of the solution.

Figure S3. HRTEM picture of **1** in 10 nm scale showing a lot of dispersed nano dotes.

Figure S4. ESI-MS of the d-T5 clusters in LiBr-DMF/MeOH solution measured after one day in ambient condition.

Table S1. Crystal data and structural refinement parameters for **1**.

1	
formula	C78H212N13Cu5In30S56
fw	6890.32
cryst size	0.22 × 0.20 × 0.12
(mm ³)	
cryst syst	Tetragonal
space group	<i>I</i> 4 ₁ /a
<i>a</i> (Å)	29.1076(13)
<i>b</i> (Å)	29.1076(13)
<i>c</i> (Å)	23.5668(19)
α (deg)	90.00
β (deg)	90.00
γ (deg)	90.00
<i>V</i> (Å ³)	19967(2)
<i>Z</i>	4
ρ_{calcd} (g cm ⁻³)	1.975
<i>F</i> (000)	10876
μ (mm ⁻¹)	4.507
<i>T</i> (K)	293(2)
reflns collected	26005
unique reflns	8786
observed reflns	3702
no. params	269
GOF on <i>F</i> ²	1.166
<i>R</i> ₁ [<i>I</i> > 2 σ (<i>I</i>)]	0.0739
<i>wR</i> ₂ for all	0.1582

Table S2. Solubility of compound **1** in different solvents with LiBr (*10 °C, 1. 0 atm, concentration of LiBr 0.20 mol/L.)

Solvent	Solubility* (mg/mL)	Solubility* (mg/100g)
ethanol	0	0
acetonitrile	0.2	25
DMSO	0.6	54
DMF	1.0	105

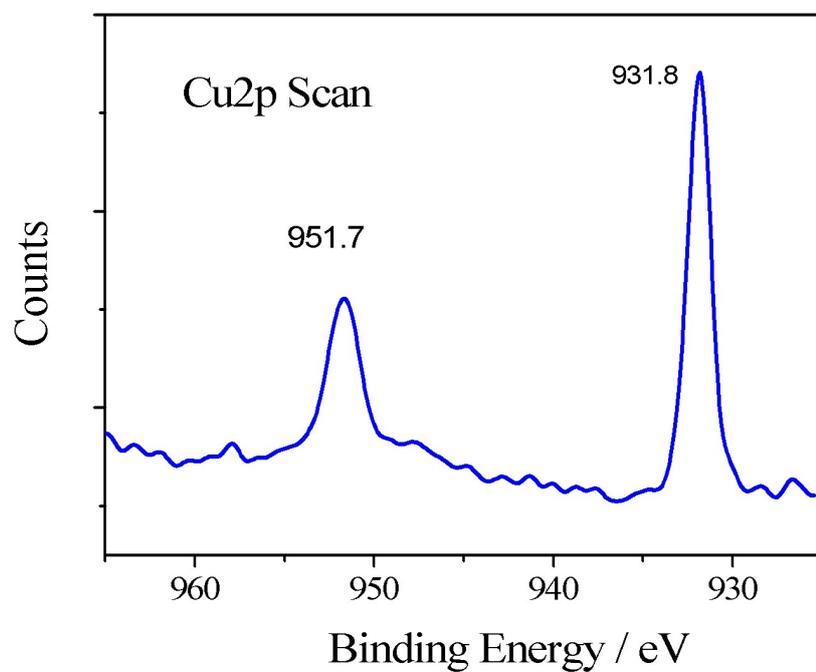


Figure S1. XPS spectra of **1**, showing the Cu2p peaks, which are in agreement with that of Cu(I).

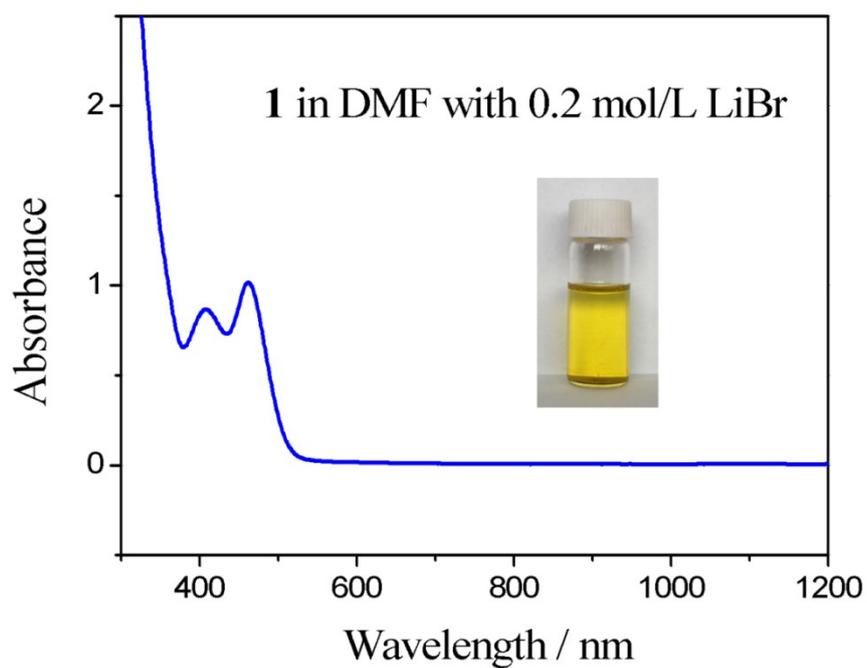


Figure S2. Absorption spectra of **1** in DMF with 0.2 mol/L LiBr. Insert is the picture of the solution.

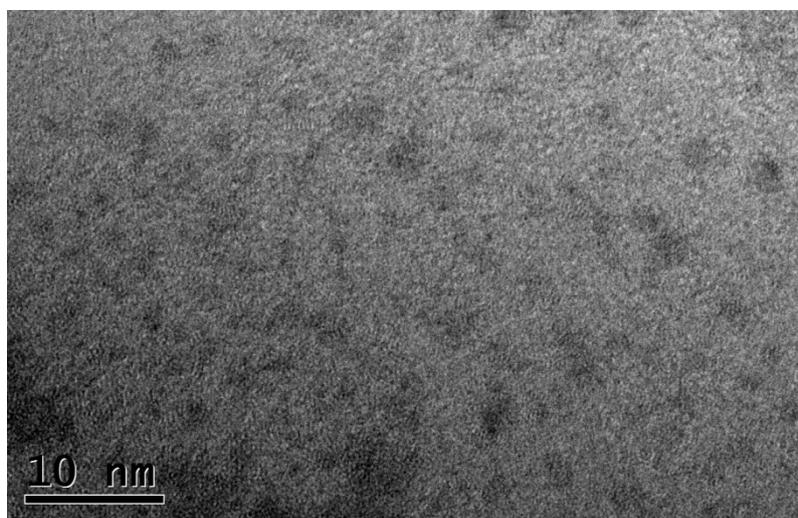


Figure S3. HRTEM picture of **1** in 10 nm scale showing a lot of dispersed nano dots.

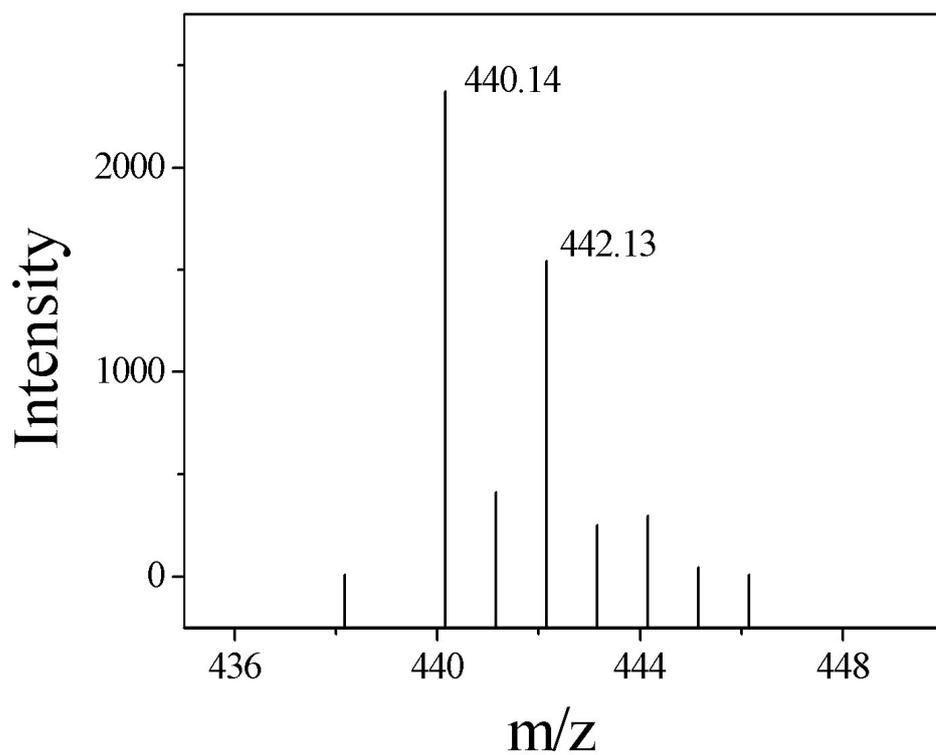


Figure S4. ESI-MS of the d-T5 clusters in DMF/MeOH solution measured after one day in ambient condition.