Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2016

Supporting Information

Multifunctional Copper Dimer: Structure, Band Gap Energy, Catalysis, Magnetism, Oxygen Reduction Reaction and Proton Conductivity

Debraj Sarkar,[a] Purna Chandra Rao,[a] Harshitha Barike Aiyappa,[b] Sreekumar Kurungot,[b] Sudip Mandal,[c] Kothandaraman Ramanujam,[c] Sukhendu Mandal[a]*

[a]School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram, Kerala, India-695016
[b]Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory (NCL), Pune, 411008, India
[c]Academy of Scientific and Innovative Research (AcSIR), New Delhi, India.
[d]Department of Chemistry, Indian Institute of Technology Madras, Chennai, 600036, India

Table S1. Crystallographic parameters for compound **1**.

Parameters	**Compound 1**
Empirical formula	$C_{17}H_{15}CuN_3O_{10}S_2$
Formula weight	548.98
Crystal System	Triclinic
Space Group	*P -1* (no. 2)
a(Å)	9.1350(4)
b(Å)	11.0789(5)
c(Å)	11.9804(5)
α(°)	92.071(2)
β(°)	94.009(2)
γ(°)	112.747(2)
Volume(Å^3)	1112.81(9)
Z	2
Calculated density, Mg/m^3	1.638
Crystal size, mm	0.12×0.10 ×0.08
θ range (deg)	2.428 to 28.378
F (000)	558
Absorption coefficient (mm^{-1})	1.228
Reflections collected	19927
Unique reflections	5544
Goodness-of-fit	1.067
Number of parameters	309
Final R indices [I>2sigma(I)]	R_1 = 0.0387, wR_2 = 0.1168
R indices (all data)	R_1 = 0.0443, wR_2 = 0.1217
Largest diff. peak and hole e Å^{-3}	0.863 and -0.733

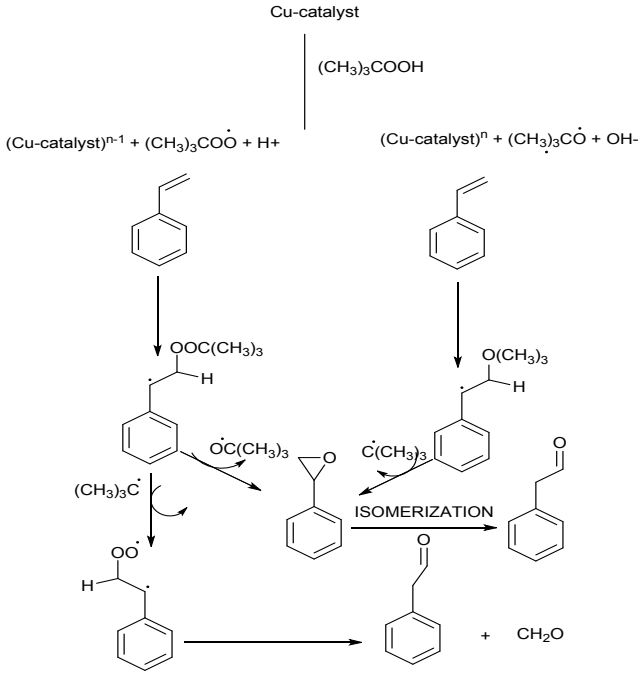
[a]$R_1 = \Sigma||F_0| - |F_c||/ \Sigma|F_0|$; $wR_2 = \{[w(F_0^2 - F_c^2)^2]/ [w(F_0^2)^2]\}^{1/2}$;

$w = 1/[\sigma^2(F_0)^2 + (aP)^2 + bP]$; $P = [\max(F_0^2,0) + 2(F_c)^2]/3$,

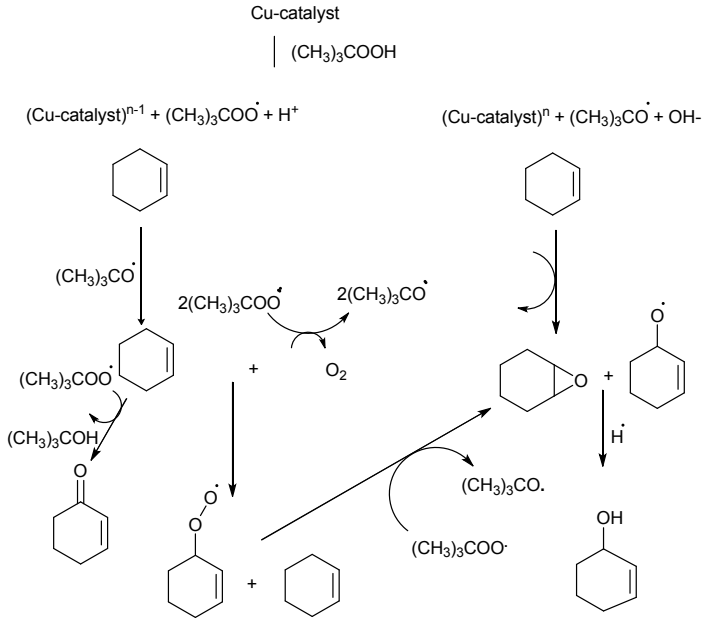
where a = 0.0702 and b = 0.8606 for compound **1**.

Table S2. Potential H-bonds in compound **1**.

Donor --- H....Acceptor	D – H (Å)	H...A (Å)	D...A (Å)	D - H...A (°)
O(2) --H(2A) ..O(1)	0.88	2.05	2.906(3)	163
O(2) --H(2B) ..O(5)	0.88	1.96	2.803(3)	158
O(200)--H(20A) ..O(3)	0.85	1.93	2.769(3)	170
O(200)--H(20B) ..O(400)	0.85	1.89	2.622(7)	144
O(200)--H(20B) ..O(500)	0.85	2.58	3.327(7)	147
C(12) --H(12) ..O(200)	0.93	2.48	3.345(4)	154



Scheme S1. Proposed mechanism for styrene oxidation.



Scheme S2. Proposed mechanism for cyclohexene oxidation.

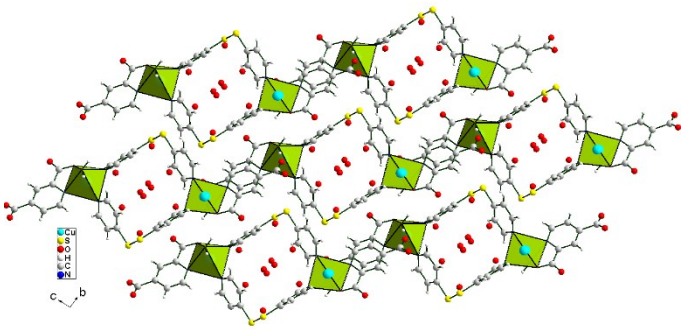
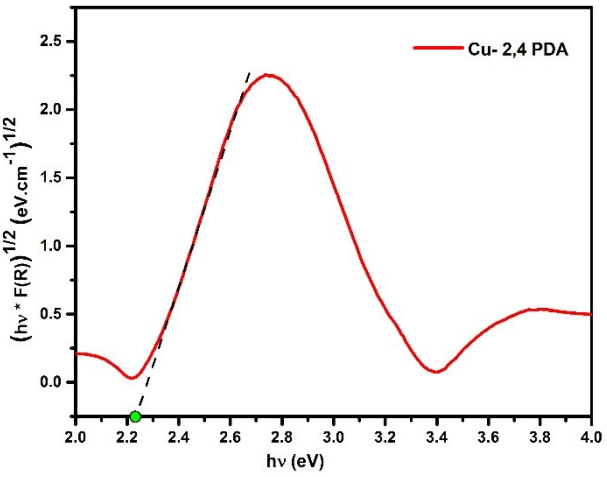
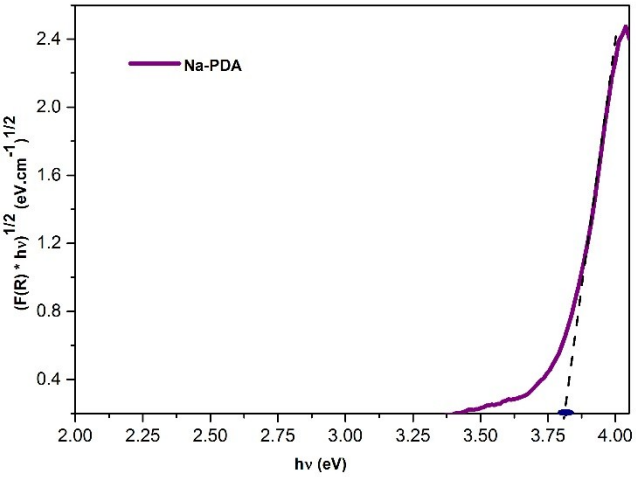


Fig. S1 The H-bonded supramolecular structure of compound **1**.

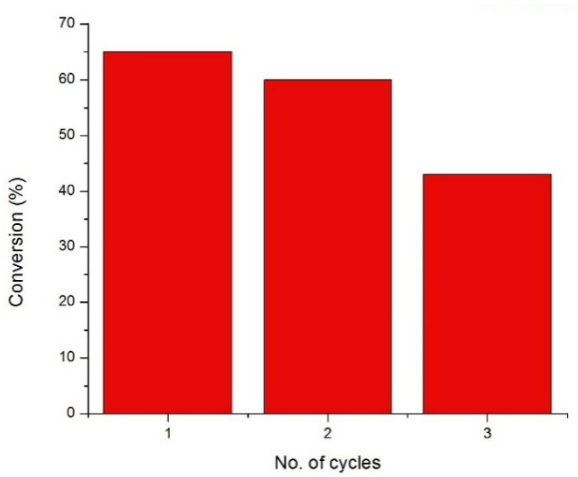


(a)

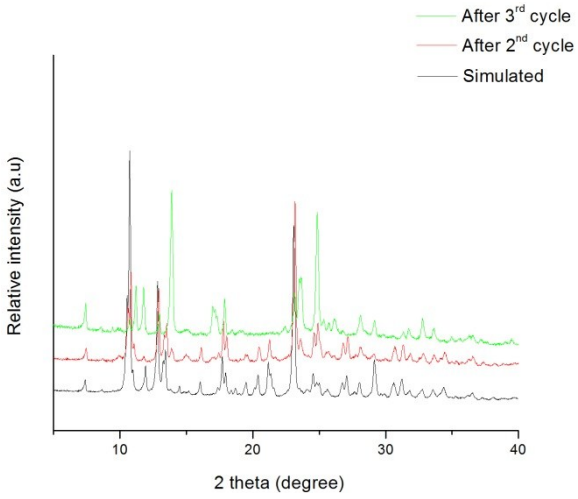


(b)

Fig. S2 Tauc plots for (a) **1** and (b) Na-salt of PDA.



(a)



(b)

Fig. S3 (a) The percentage of product conversion after each catalytic cycles. (b) The PXRD pattern of the catalyst after each cycles.

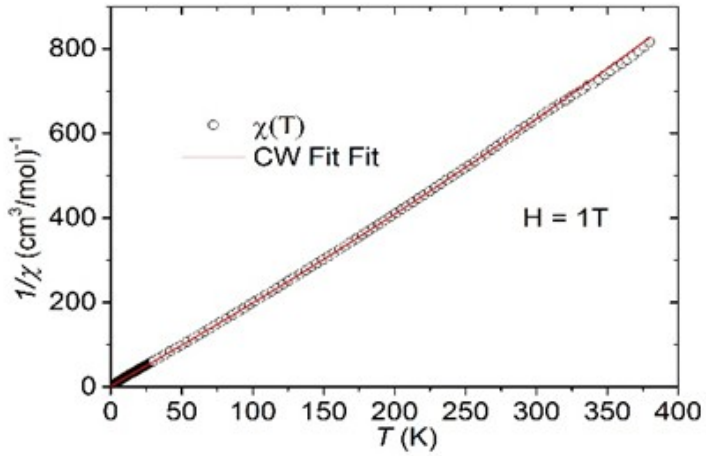


Fig. S4 1/χ data of compound **1** (solid line represent the Currie-Weiss fitting).

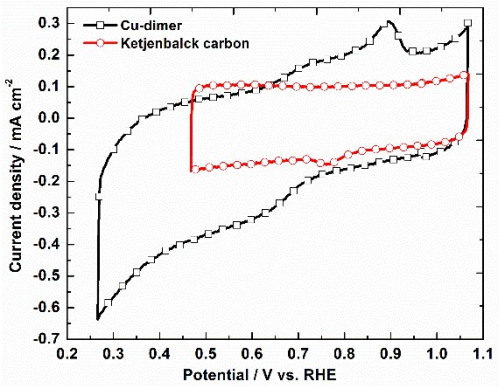


Fig. S5 Cyclic voltammetry recorded in N_2 saturated 0.1 N KOH solution for Cu-dimer/C and Ketjenblack carbon.

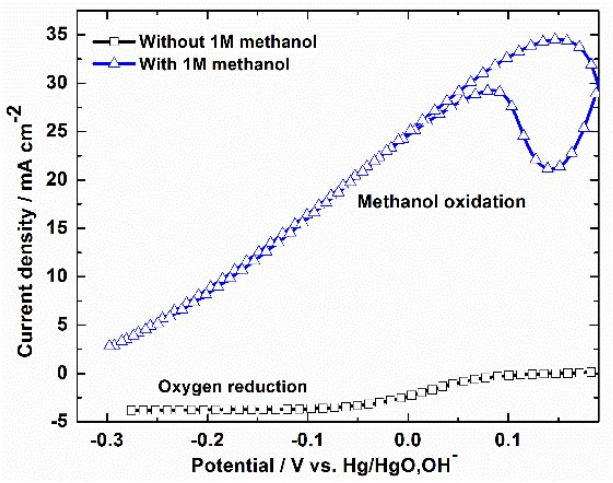


Fig. S6 Polarization curves obtained in 0.1 N KOH solution with and without 1M methanol for Pt/C.

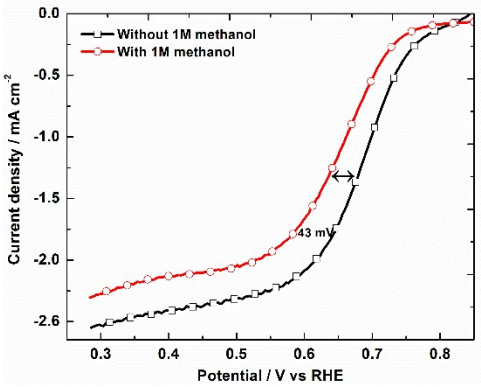


Fig. S7 Polarization curves obtained in 0.1 N KOH solution with and without 1M methanol for Cu-dimer/C.

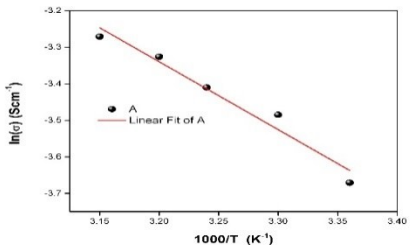


Fig. S8 Arrhenius plot for temperature dependence of conductivity at 100 % RH.

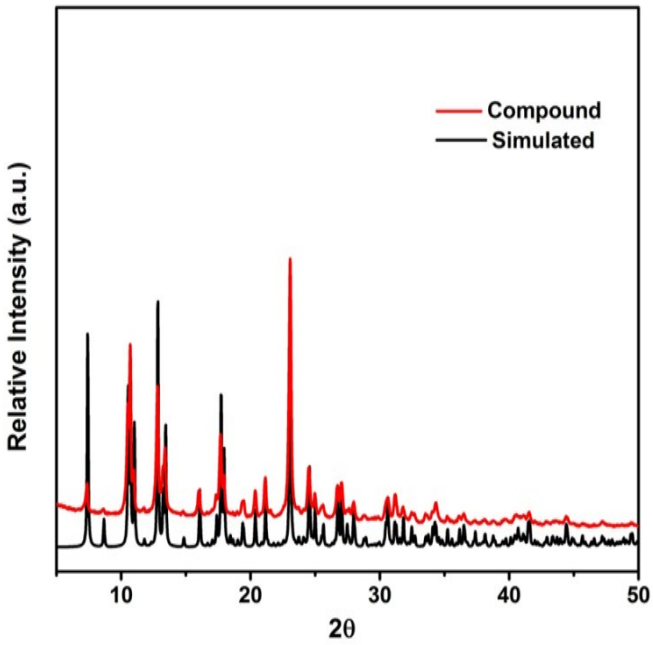


Fig. S9 The simulated and experimental powder X-ray diffraction patterns of compound **1**.

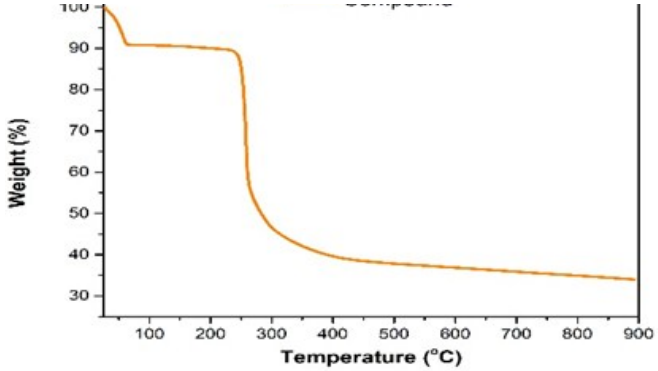


Fig. S10 Thermogravimetric analysis plot of compound **1**.

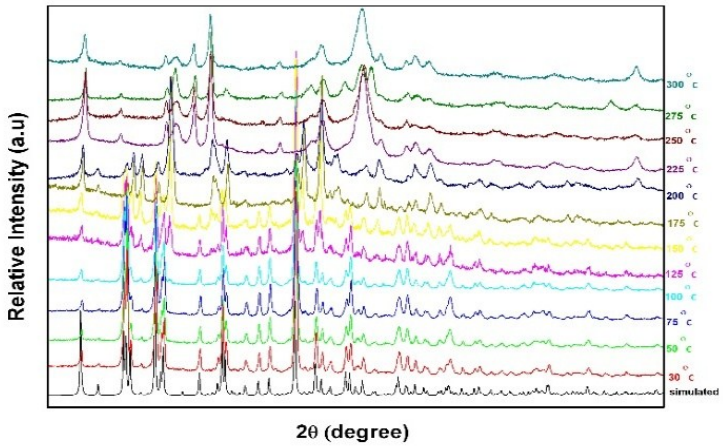


Fig. S11 The PXRD pattern of compound **1** at different temperatures. Note: compound is stable upto 250 ºC.

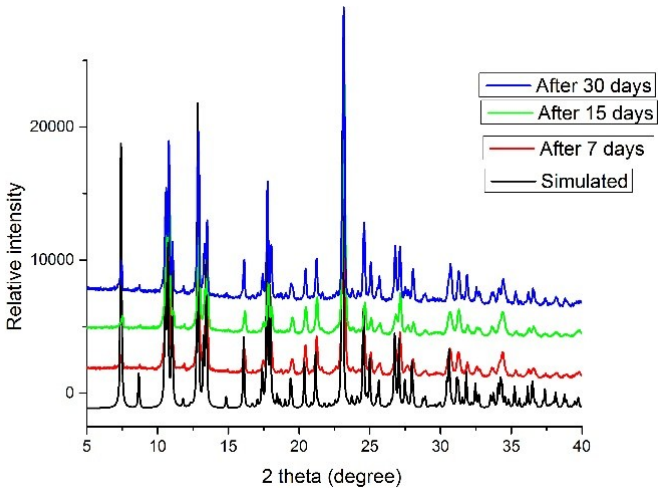


Fig. S12 The PXRD pattern of compound **1** after soaking in water. Note: compound is stable even after 30 days also.

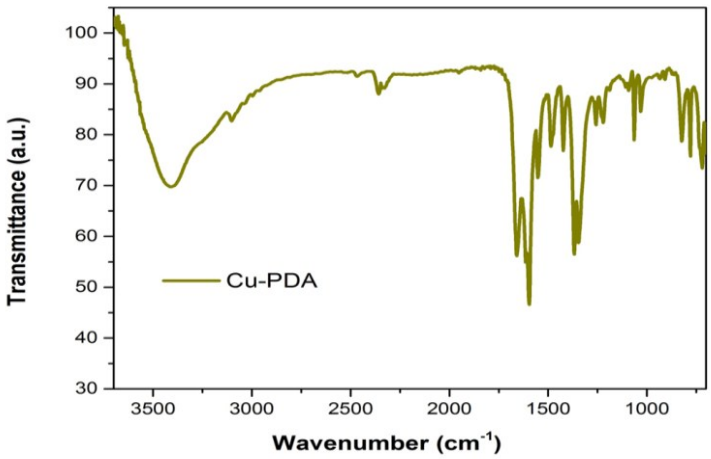


Fig. S13 The Infrared Spectrum of compound **1**.