Synergistic impact of nano-supramolecular coordination polymer based on cadmium, ethyl nicotinate and thiocyanate ligands as efficient catalyst to remove harmful elements from wastewater.

By

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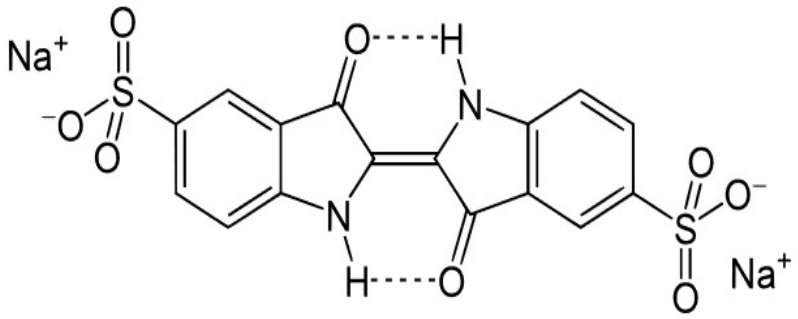
Supplementary Materials



Scheme S1 Chemical structure of Indigo carmine dye (IC).

Table S1 The SCP **1**'s crystal data and structural refinement parameters.

	1
Empirical Formula	$C_{18}H_{18}N_4O_4S_2Cd$
Formula Weight g/mol	530.894

Temperature (K)	298
Crystal system	Monoclinic
Space group	$P2_1/c$
Crystal size	0.51×0.32×0.16 mm
a/Å	5.7859 (2)
b/Å	15.7906 (7)
c/Å	12.0818 (5)
α/°	90.00
β/°	95.403 (2)
γ/°	90.00
V/Å^3	1098.92 (8)
Z	2
μ(Mo-Kα)/m.m^{-1}	2.14
Calculated density/ mg.cm^{-3}	1.604
Goodness-of-fit on F^2	0.989
F(000)	532
R indices[I>3σ(I)] R1/wR2	0.0390/ 0.1341
R indices(all data)	0.0390/ 0.1068
Data / restraints / parameters	4744/0/130
CCDC	1527036

Table S2 Bond lengths (Å) and bond angles (deg.) of the SCP **1.**

Cd1—N4^{i}	2.318 (2)	N4^{i}—Cd1—N4^{ii}	180.00 (10)
Cd1—N4^{ii}	2.318 (2)	N4^{i}—Cd1—N16	89.01 (9)
Cd1—N16	2.398 (2)	N4^{ii}—Cd1—N16	90.99 (9)
Cd1—N16^{iii}	2.398 (2)	N4^{i}—Cd1—N16^{iii}	90.99 (9)
Cd1—S2	2.7291 (8)	N4^{ii}—Cd1—N16^{iii}	89.01 (9)
Cd1—S2^{iii}	2.7291 (8)	N16—Cd1—N16^{iii}	180.00 (13)
S2—C12	1.6312 (7)	N4^{i}—Cd1—S2	93.65 (7)
C3—N16	1.342 (4)	N4^{ii}—Cd1—S2	86.35 (7)
Cd1-Cd1^{i}	5.786(8)	N4^{i}—Cd1—S2^{iii}	86.35 (7)
Cd1-Cd1^{iii}	14.554(4)	N4^{ii}—Cd1—S2^{iii}	93.65 (7)

Symmetry codes: (i) -x,y,1/2-z; (ii) -x,-y,1-z; (iii) x,-y,z-1/2;

Table S3 Hydrogen bond lengths (Å) and bond angles (deg) of the SCP **1.**

D-H….A	d(D-H)	d(H….A)	d(D….A)	∧(DHA)
C9-H9……S2	0.960	2.824	3.392	118.76
C6-H6……N3	0.960	2.844	3.333	112.60
C15-H15A……N3	0.960	2.947	3.780	145.80
C13-H13……S2	0.960	3.006	3.875	151.33

C12-H12…..S2	0.960	3.0541	3.733	128.97
C15-H15C……S2	0.960	3.196	4.107	159.12

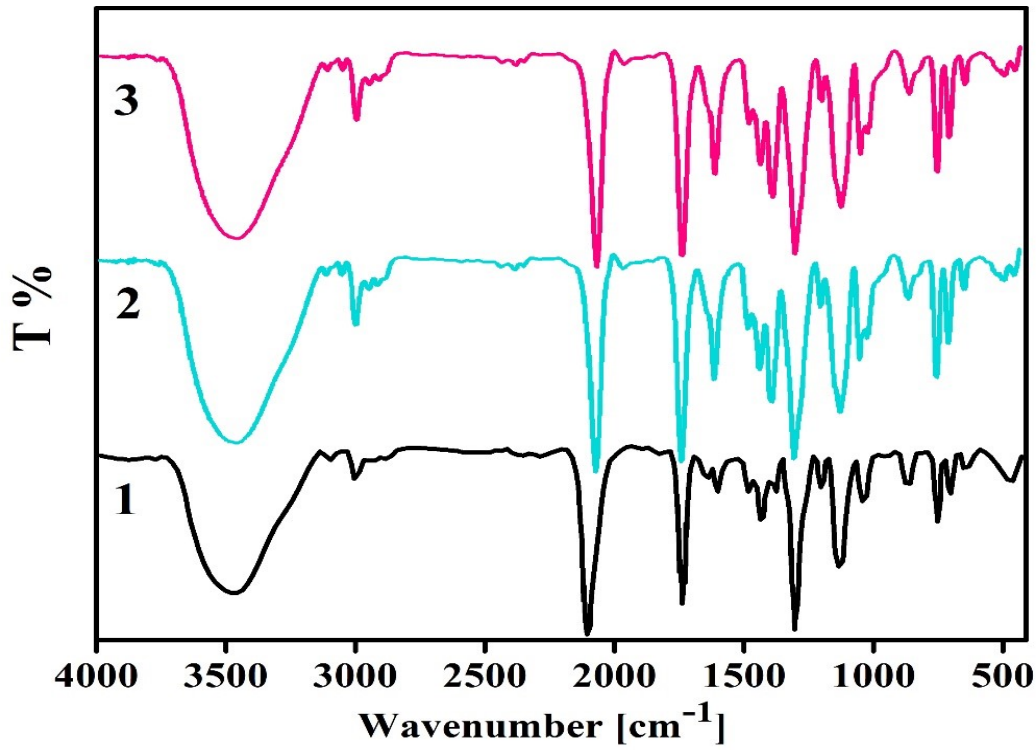


Figure S 1 IR spectra of SCP**1** (1), NSCP**1** (2) before, and after catalysis (3).

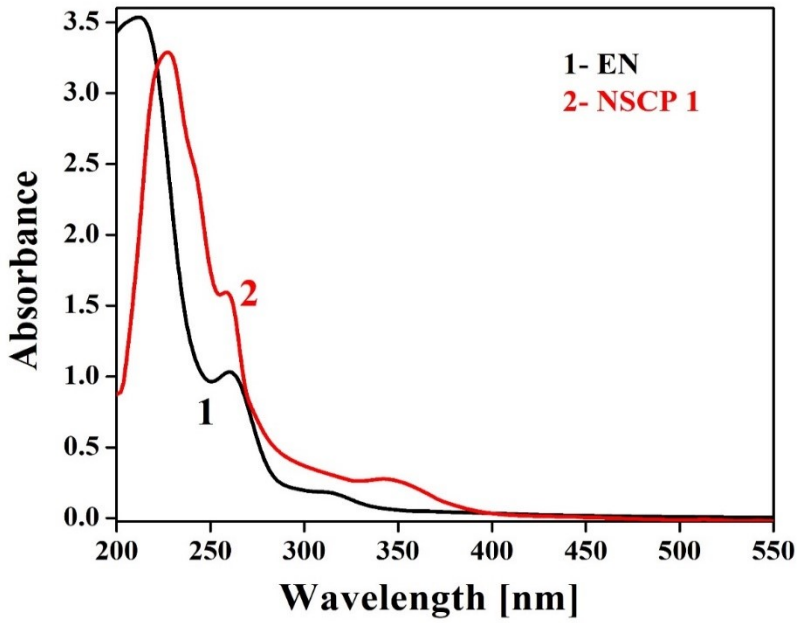


Figure S2 UV-spectra of EN and NSCP**1**

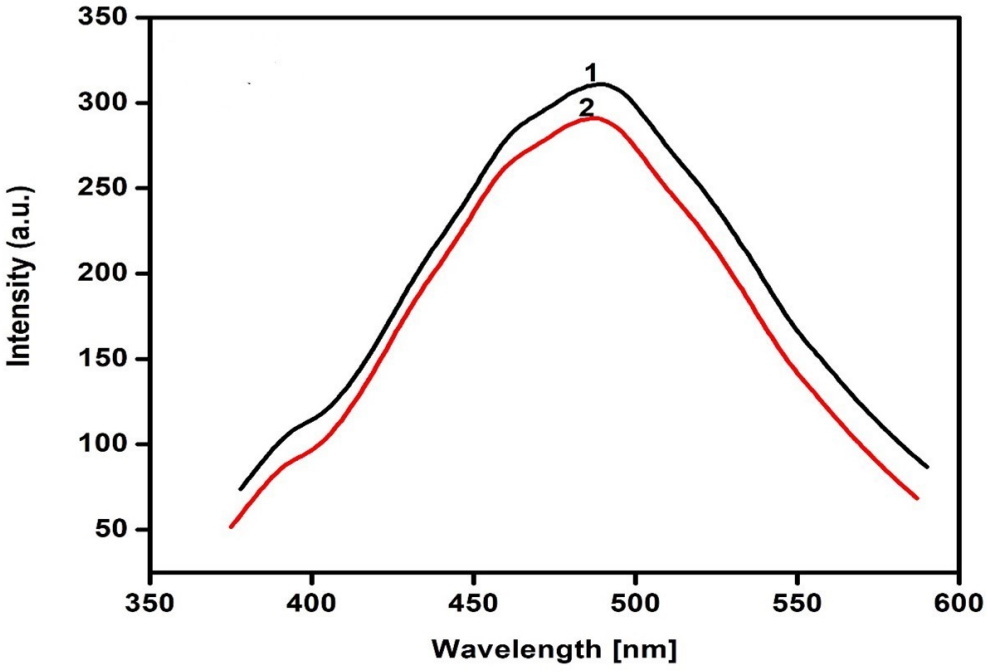


Figure S3 Emission-spectra of (1) SCP**1** and (2) NSCP**1**

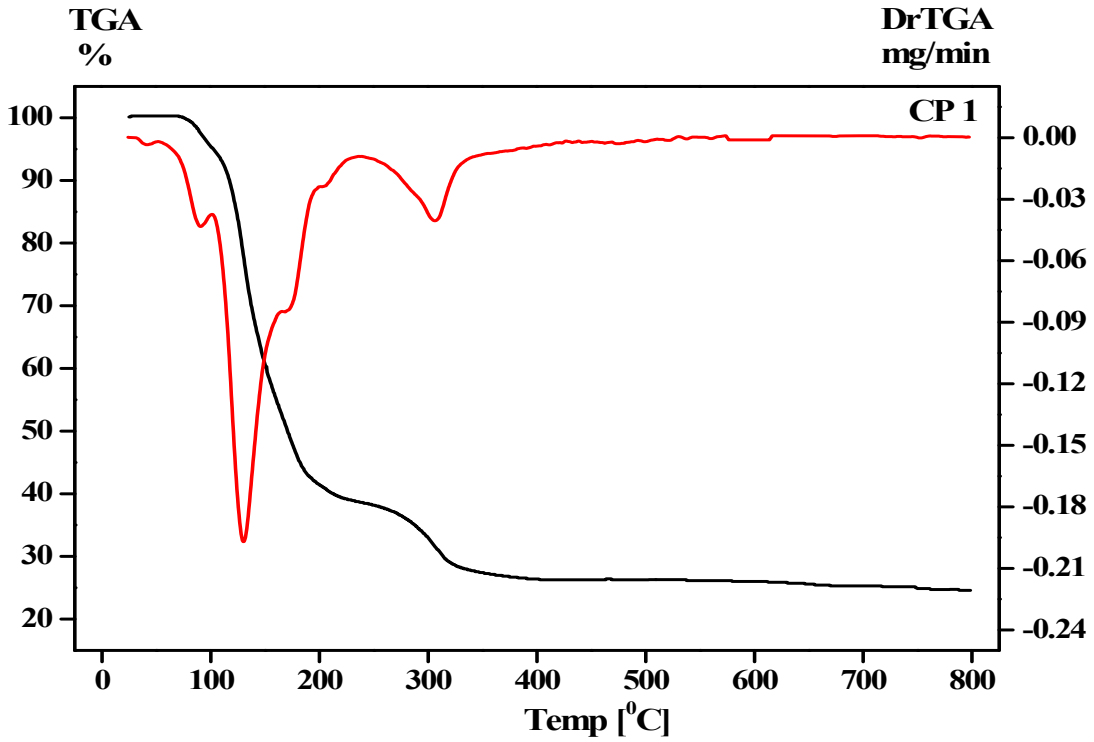


Figure S 4 TGA and DTG thermal analysis curves of the NSCP **1.**

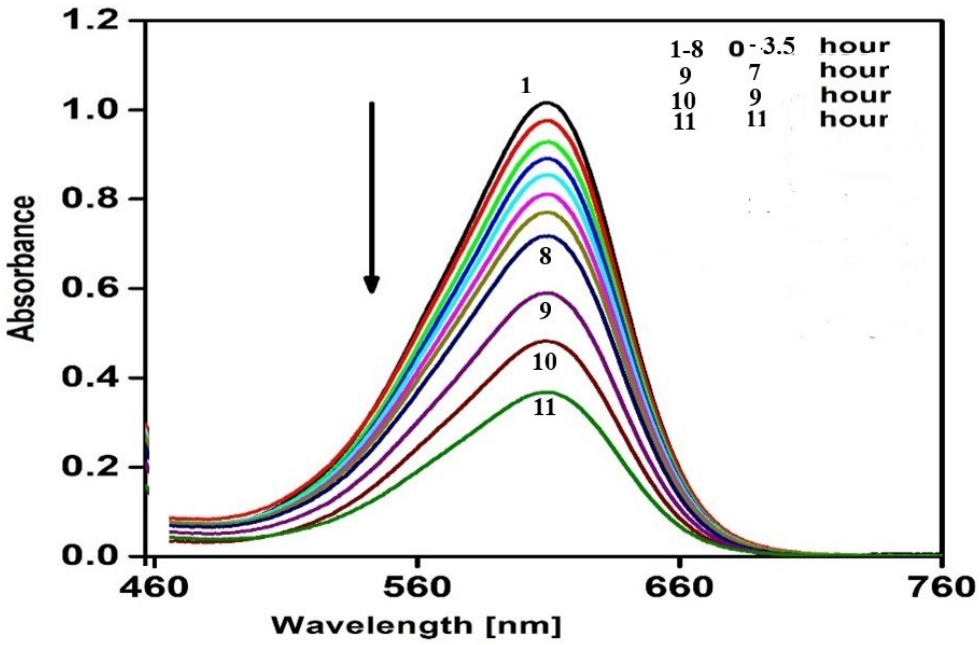


Figure S 5 Control spectra of degradation of the IC dye solution (7.0×10^{-5} M) under UV-light irradiation.

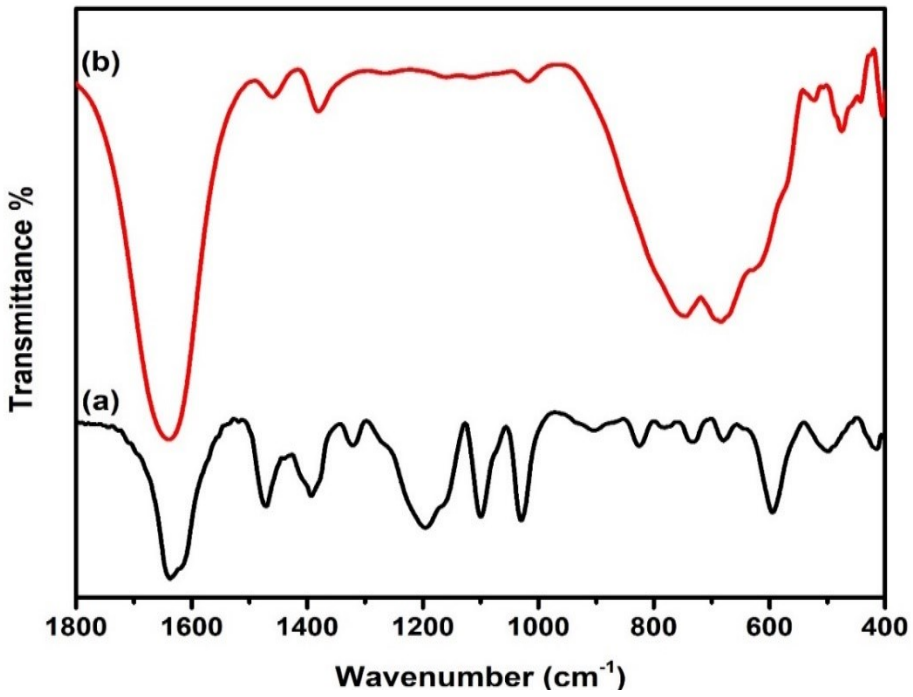


Figure S6 Indigo carmine dye (IC) infrared spectra (a) prior to and (b) after degradation.

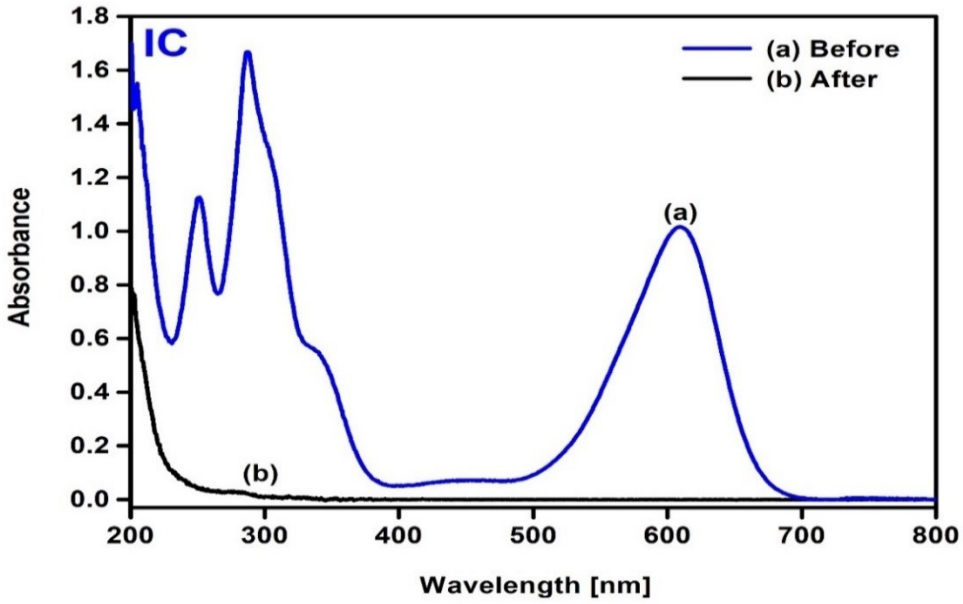


Figure S7 The electronic absorption spectra of Indigo carmine dye (IC) (**a**) before and (**b**) after degradation.

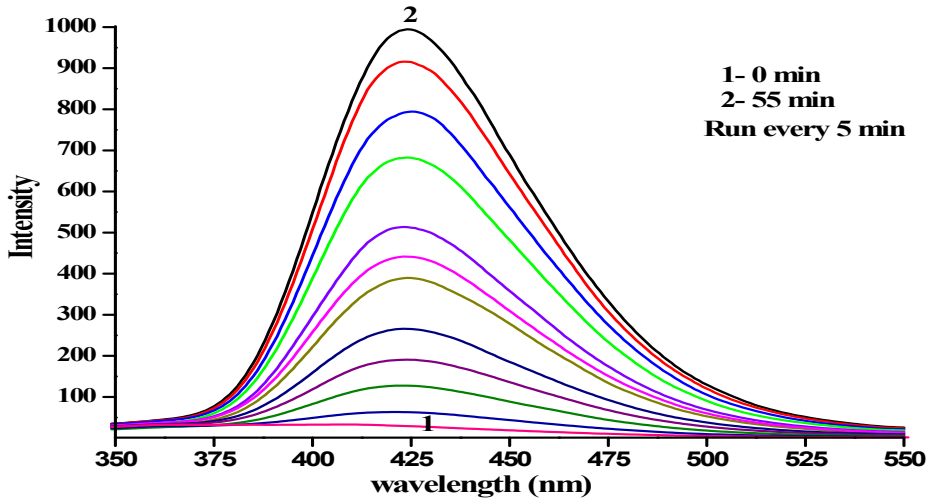


Figure S8 SCP**1** (25 mg), NaTA (0.05 M), and H_2O_2 (0.1 M) photoluminescence spectra as a function of time.

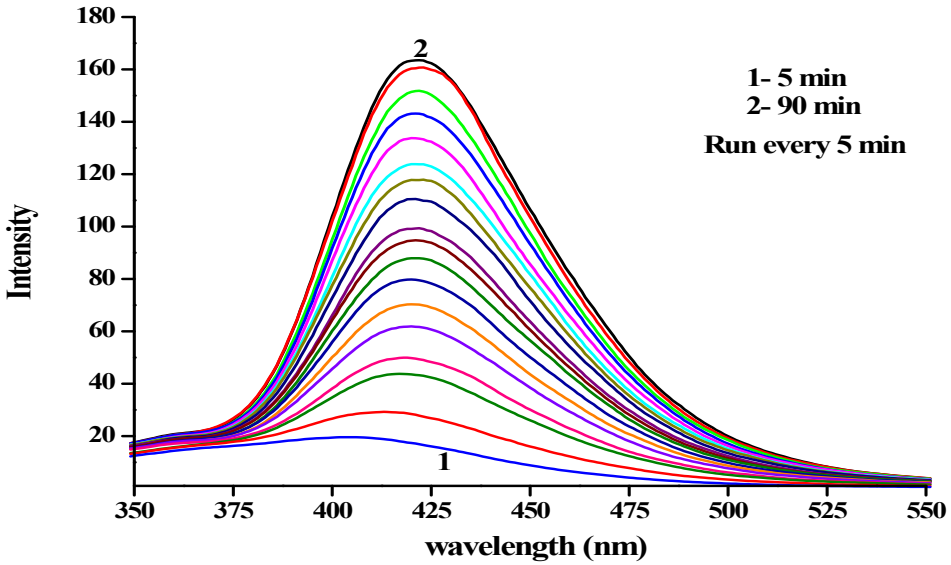


Figure S9 Photoluminescence spectra of the SCP**1** (25 mg), indigo carmin ($7{,}0x10^{-5}$ M), NaTA (0.05 M) and H_2O_2 (0.1M) as function of time