Supplementary information

Polyoxometalate nanocluster-infused triple IPN hydrogels for excellent microplastic removal from contaminated water: detection, photodegradation, and upcycling

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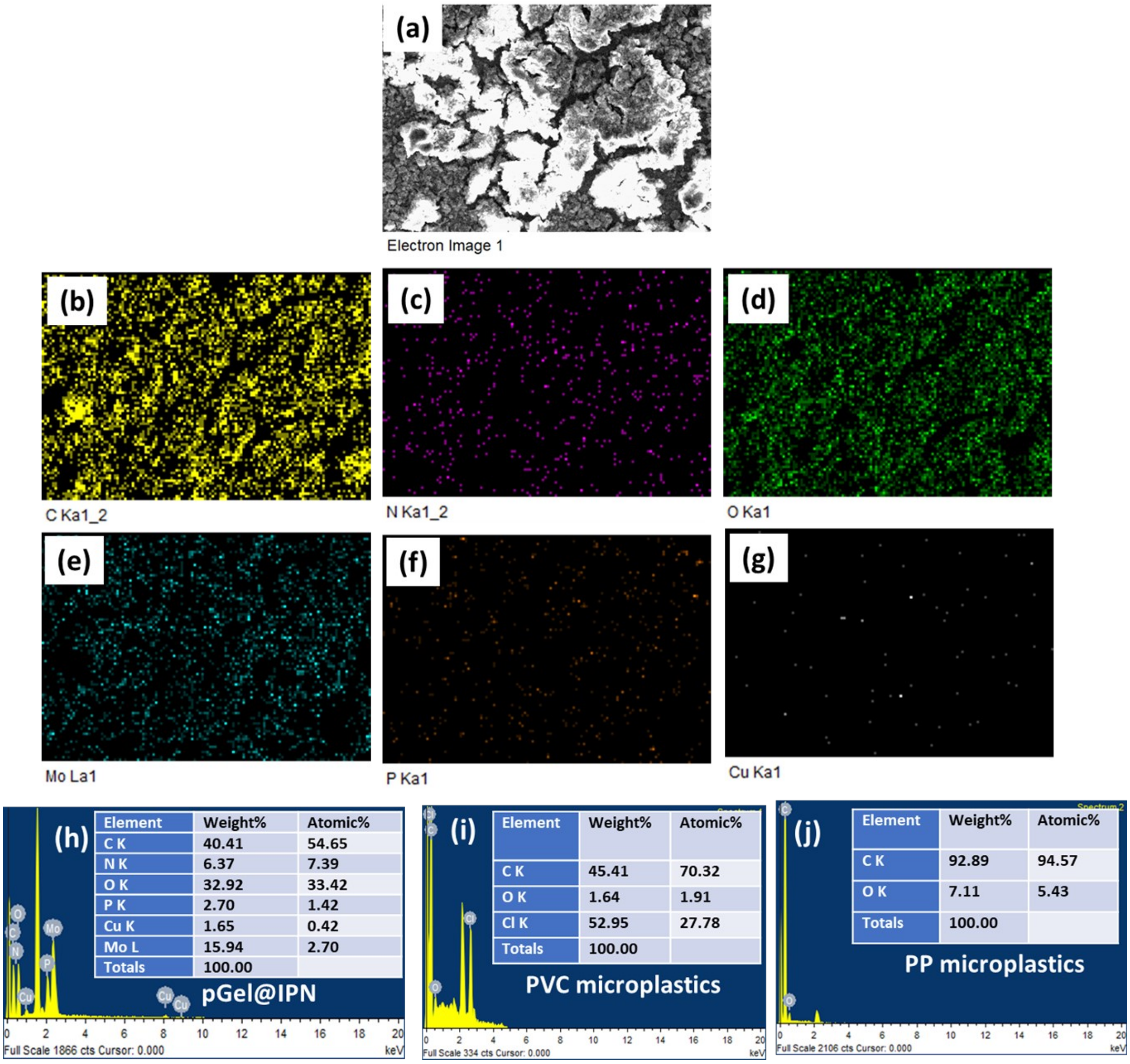
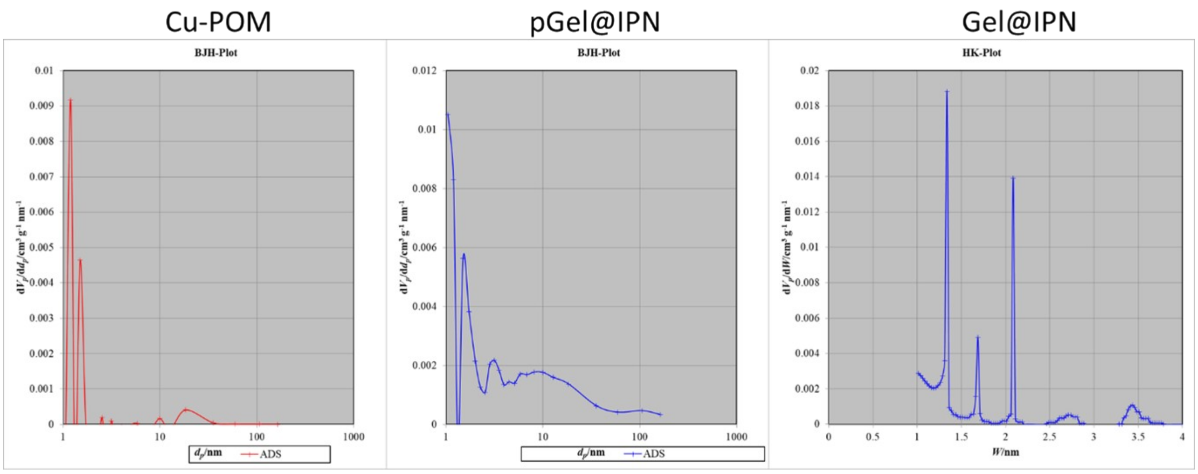


Fig. S1 (a-f) Electronic SEM images and elimental maping of pGel@IPN hydrogel, respectively; EDX spectrum and composition of (g) pGel@IPN hydrogel, (h) PVA microplastic, and (j) PP microplastic.



BET analysis Parameters	Cu-POM	pGel@IPN	Gel@IPN
BET surface area, $a_{s,BET}$ [$m^2\ g^{-1}$]	0.4629	35.113	3.0823
Average pore diameter [nm]	32.691	12.464	1.4719
Average Pore Volume [$cm^3\ g^{-1}$]	0.003783	0.1094	0.0022685

Fig. S2 the pore size distribution plot for Cu-POM, pGel@IPN, and Gel@IPn, illustrating their respective structural characteristics. Additionally, the BET (Brunauer-Emmett-Teller) analysis parameters for these materials are summarized in the accompanying table.

Text S1: Water Contact Angle

The water contact angle (WCA) is a crucial parameter assessing the surface wettability of prepared hydrogel, commonly employed to evaluate hydrophilicity and hydrophobicity. We used the sessile drop method in a goniometer to determine the WCA. A surface with a WCA less than 90° is classified as hydrophilic, indicating an affinity for water, while a high contact angle (>90°) suggests hydrophobicity, repelling water. In this study, the WCA of the IPN hydrogel matrix system was measured [1]. Detailed contact angle analysis focused on the position and angle of the contact angle is displayed in Fig. 4f (manuscript). For the prepared hydrogel, a WCA of ~50º ± 2º indicates a strong affinity for water, signifying a hydrophilic hydrogel surface. The enlarged view of the WCA for the pGel@IPN hydrogel surface is illustrated in the manuscript, Fig. 4f, inset. Conventionally, the contact angle is measured from the liquid side, representing the angle a liquid creates with an ideal solid surface with specific characteristics. This definition captures the intricate interplay between surface characteristics and liquid interactions.

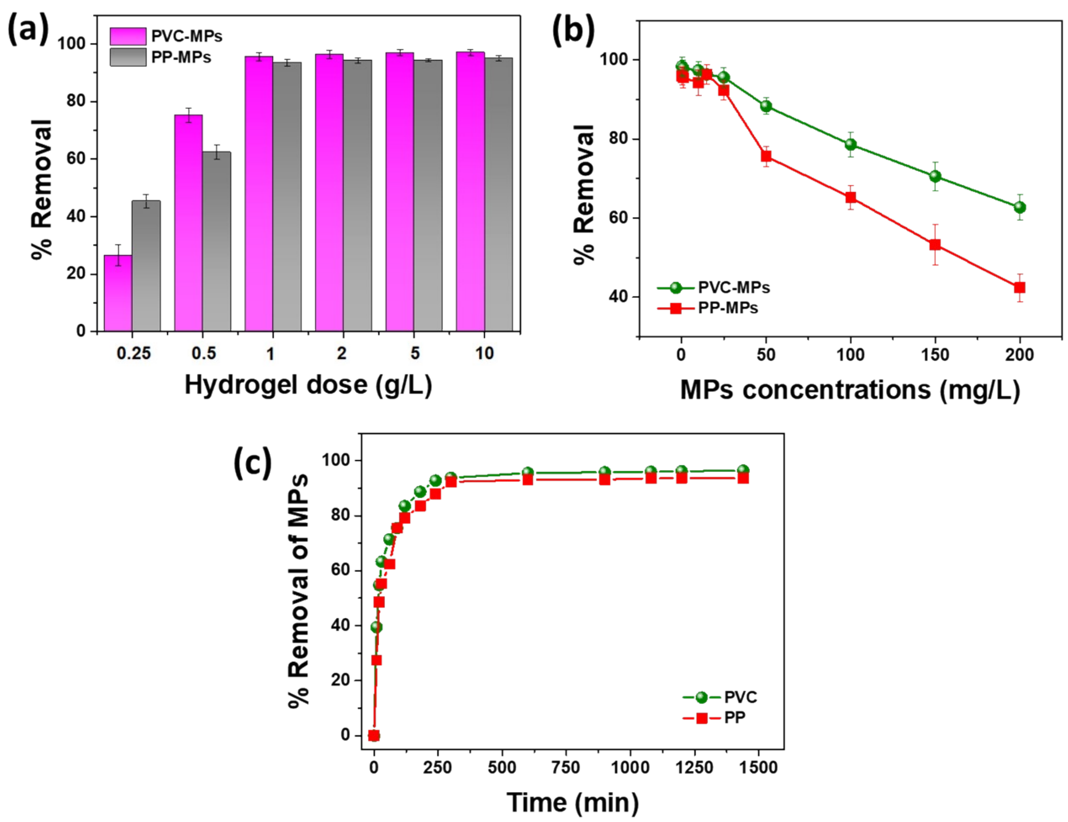


Fig. S3 Microplastic removal efficiency by varying different (a) hydrogel dose, (b) Microplastics concentrations and (c) contact time. (Experimental condition: contact time: 300 min, initial concentration of MPs: 25 mg/L; pGel@IPN hydrogel dose: 1g/L)

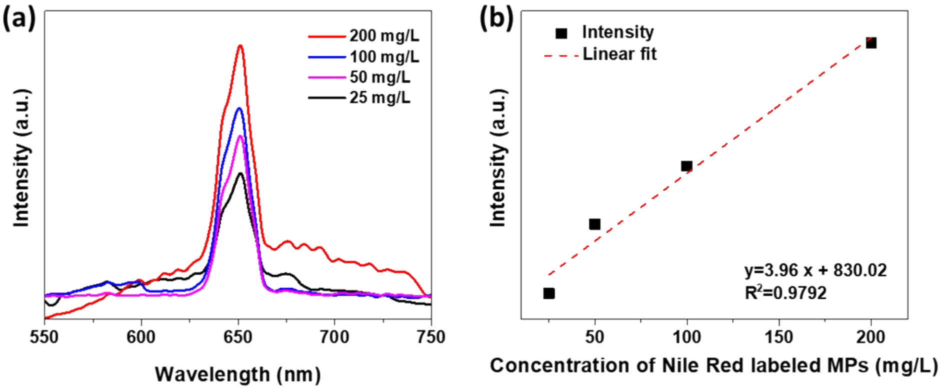


Fig. S4 (a) The fluorescent Nile red dye-tagged PVC-MPs with varying concentrations and their corresponding wavelengths. (b) the graph showcases the calibration curve fitted for the detection of microplastics, providing an analytical framework for quantifying microplastic concentrations based on fluorescence intensity.

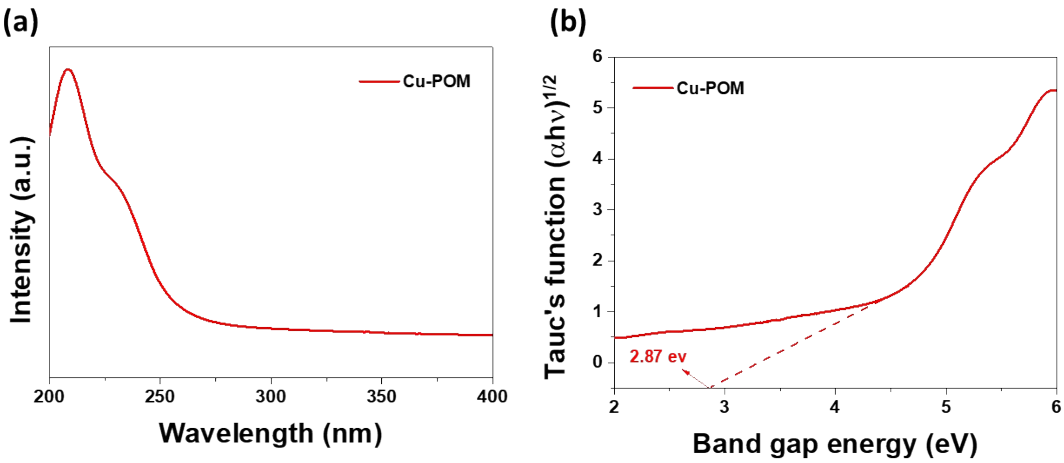


Fig. S5 (a) UV–vis spectra of Cu-POM nanocluster in water, (b) respective band gap energy (Eg) determination from the Tauc plot.

Text S2: Tauc plot for band gap energy determination of Cu-POM nanocluster

The Tauc plot is a graphical method used for determining the band gap energy of a material from its absorption spectrum. here we have tried to evaluate the band gap energy of the catalyst Cu-substitute polyoxometalate (Cu-POM). The formula for the Tauc plot is given by $(\alpha h\nu)^{1/n} = A(h\nu - E_g)$, where A is a constant, E_g is the band gap energy, h is Planck's constant, ν is the photon frequency and n depends on the nature of the electronic transition if n = 2 (for direct band gap) or n = 1/2 (for indirect band gap). It involves plotting the $(\alpha h\nu)^{1/n}$ against the photon energy (hν). The plot typically exhibits a linear region, and extrapolating the linear portion to the energy axis allows for the determination of the band gap energy.

Table S1. Kinetic parameters for PVC and PP microplastic adsorption on pGel@IPN hydrogel

Kinetic models		**Parameters**	**PVC-MPs**	**PP-MPs**
Pseudo second-order model		qe (mg g^{-1})	48.47523	47.8455
		K_2 (min^{-1})	0.00123	0.0008
		R^2	0.99173	0.98547
		Adj. R^2	0.9911	0.98426
		Root-MSE (SD)	1.29567	1.31272
Intra-particle diffusion model	1st stage	C (mg/g)	5.87315	1.90498
		K_d (mg/g $min^{-0.5}$)	0.42586	17.66838
		Adj. R^2	0.99479	0.91553
		Root-MSE (SD)	2.04678	9.00283
	2nd stage	C (mg/g)	1.63801	5.18658
		K_d (mg/g $min^{-0.5}$)	22.81023	-0.57365
		Adj. R^2	0.97872	0.97488
		Root-MSE (SD)	1.59595	7.79743
	3rd stage	C (mg/g)	0.11824	0.15333
		K_d (mg/g $min^{-0.5}$)	44.1475	41.72955
		Adj. R^2	0.67822	0.56458
		Root-MSE (SD)	3.33563	8.77025

Table S2. Isotherm parameters for PVC and PP microplastic adsorption on POM-HG@IPN hydrogel

Isotherm models	Parameters	PVC-MPs	PP-MPs
Langmuir isotherm	Q_m (mg/g)	321.86927	144.29208
	b (L/mg)	0.00322	0.00769
	R^2	0.99989	0.99706
	Adj. R^2	0.99988	0.99664
	Root-MSE (SD)	0.52797	1.94359
Freundlich isotherm	K_f [(mg/g)(L/mg)$^{1/n}$]	2.04517	3.06172
	1/n	1.27844	1.56157
	R^2	0.99714	0.98512
	Adj. R^2	0.99673	0.98299
	Root-MSE (SD)	2.69965	4.37094

Table S3. Thermodynamics parameter for PVC dye and PP microplastic adsorption on pGel@IPN hydrogel.

Dye	Temperature (K)	ΔG° (kJ/mol)	ΔH° (kJ/mol)	ΔS° (kJ/mol K)	R^2
PVC-MPs	293	-4.0467	27.33548	0.10735	0.96433
	303	-5.33974			
	313	-6.18373			
PP-MPs	293	-7.7993	67.87938	0.25845	0.99845
	303	-10.53341			
	313	-12.96161			

References

1 T. Huhtamäki, X. Tian, J. T. Korhonen and R. H. Ras, *Nature protocols*, 2018, **13**, 1521–1538.