Electronic Supplementary Material (ESI) for Dalton Transactions.

Polymer modified mesoporous silica microcubes (P@MSMCs) for synergistic oxidative entrapment of Ag(I), Ti(IV) and Zn(II) from natural river water

Shanaz Jahan[a*], Muhammad Salman[b], Yatimah Binti Alias[cd*], Ahmad Farid Bin Abu Bakar[a], Farrukh Mansoor[e], Shamsa Kanwal[e]

[a] Department of Geology, Faculty of Science, University of Malaya, Kuala Lumpur 50603, Malaysia.

[b]Department of Polymer Engineering, Xian Jiaotong University, Shanxi province, China.

[c] Department of Chemistry, Faculty of Science, University of Malaya, Kuala Lumpur 50603, Malaysia.

[d] University Malaya Centre for Ionic Liquids (UMCiL), University of Malaya, Kuala Lumpur 50603, Malaysia.

[e] Department of Chemistry, Khawja Fareed University of Engineering and Information Technology, Rahim Yar Kahan, Pakistan.

Corresponding author e-mail: jshanaz01@gmail.com, yatimah70@um.edu.my

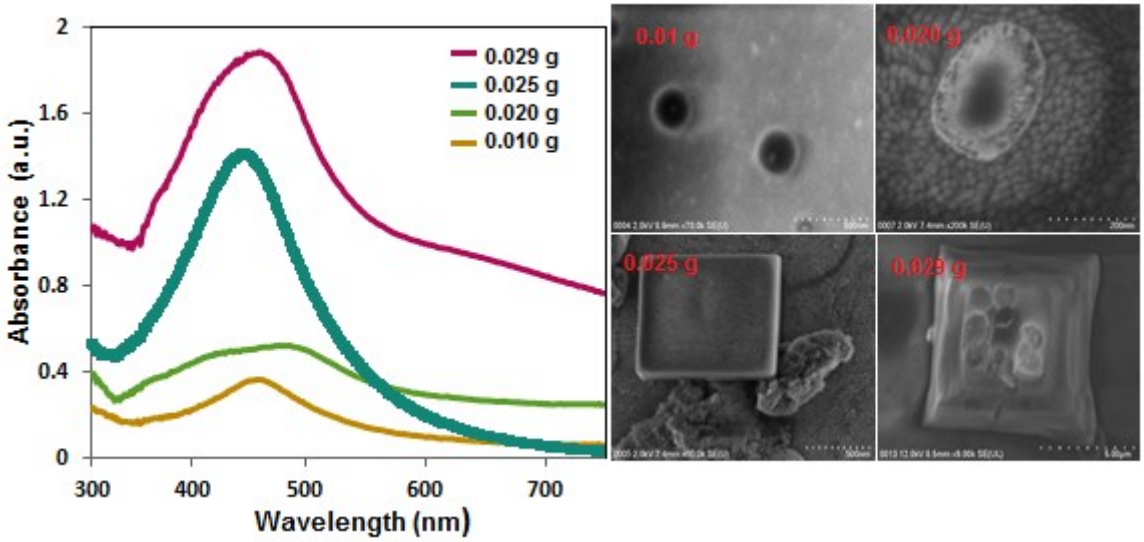

Figure S1: The UV-visible and FESEM analysis for the optimization of $FeCl_3$ concentration during the synthesis of P@SMCs.

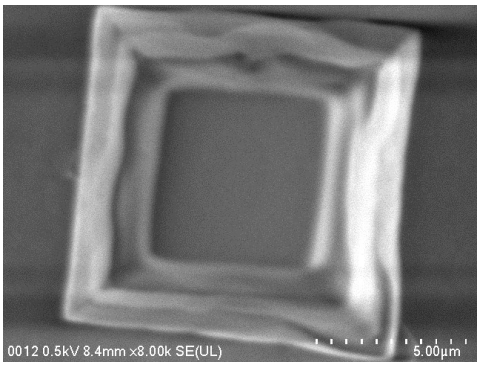

Figure S2: FESEM image of P@SMCs with polymer layer at the surface.

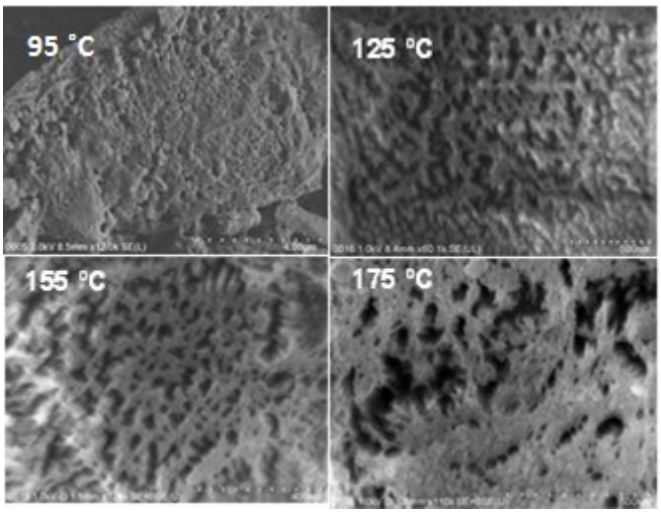

Figure S3: Porosity control of P@MSMC at different temperature values.

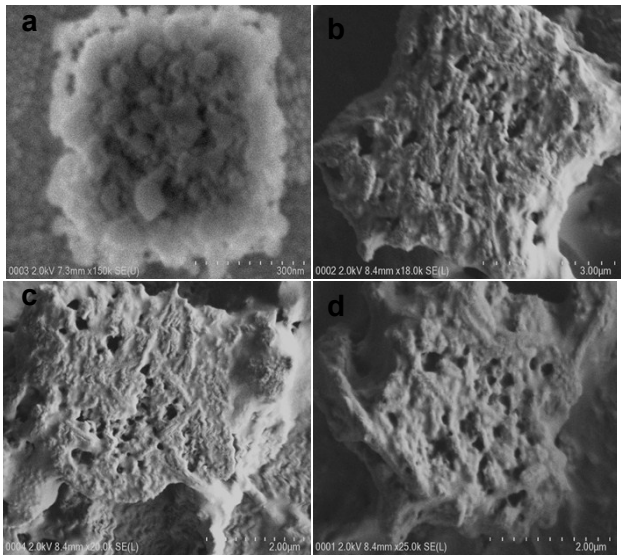

Figure S4: The corresponding FESEM images of the disintegration of polymer layer at temperature 170 ˚C (a), 180 ˚C (b), 190 ˚C (c) and 200 ˚C.

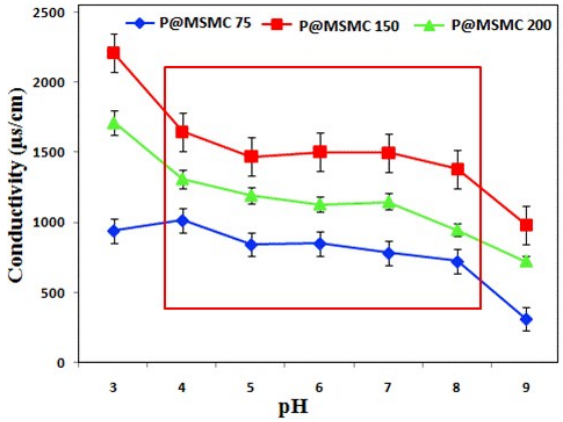

Figure S5: The stability of P@MSMC (synthesize at 75 ˚C, 150 ˚C & 200 ˚C) at variable solution pH. The error bars representing the standard error of three replicate analysis.

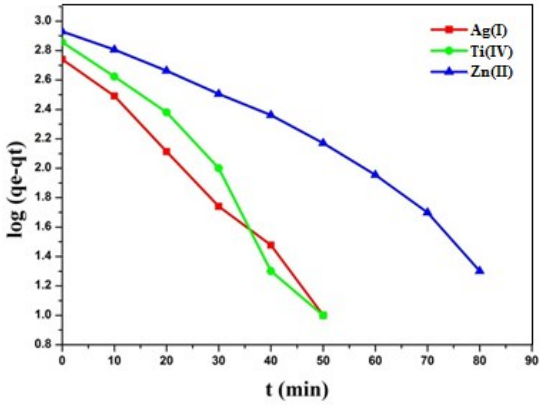

Figure S6: The Pseudo-first-order kinetics plots for metal ions adsorption on P@MSMC (R^2 value = 0.993, 0.964 and 0.966 for Ag, Ti and Zn, respectively.

Table S1*. The physical characteristics and ionic composition of natural River water.

Physical Parameters		
pH	**DO (mg/L)**	**TSS (mg/L)**
6.86 ± 0.04	11.5 ± 0.02	100 ± 0.53
Ionic Composition (mg/L)		
Anions	Fluoride	0.364 ± 0.01
	Chloride	34.15 ± 0.61
	Carbonate	30.47 ± 0.01
	Bromide	0.998 ± 0.03
	Nitrate	4.504 ± 0.21
	Phosphate	2.194 ± 0.02
	Sulfate	36.32 ± 0.03
Cations	Sodium	31.70 ± 0.11
	Potassium	50.17 ± 0.02
	Calcium	26.11 ± 0.04
	Magnesium	41.05 ± 0.02

*All values are recorded at 28 ˚C using portable meter.

Table S2: Pseudo-first-order and pseudo-second-order kinetic model constants of as-prepared P@MSMC

Metal ions	$q_{e.}$exp (mgg^{-1})	Pseudo-first order model				Pseudo-first order model			
		$q_{e.}$exp (mgg^{-1})	K_1 (x 10^{-2} min^{-1})	R^2	RMSE (%)	$q_{e.}$exp (mgg^{-1})	K_1 (x 10^{-3} mg^{-1} min^{-1})	R^2	RMSE (%)
Ag	520	436	0.15	0.993	21.3	519	1.1	0.999	0.23
Ti	720	648	0.11	0.964	53.2	722	7.6	0.999	4.5
Zn	850	763	0.12	0.966	8.2	852	4.2	0.998	1.9

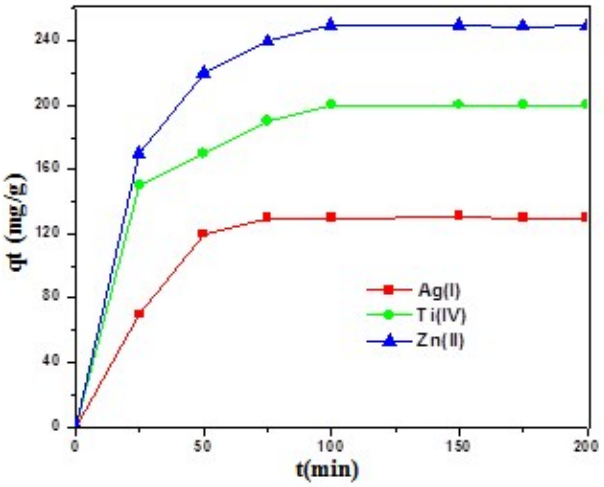

Figure S7: Adsorption potential of iron-free spherical silica structure for Ag(I), Ti(IV) and Zn(II) at 28 ˚C and at pH values 5, 6, and 6, respectively.

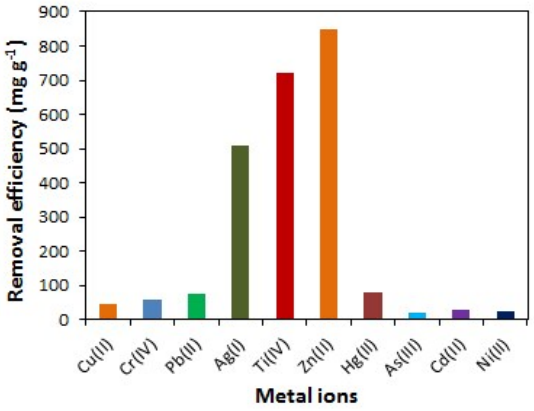

Figure S8: Adsorption efficiency of P@MSMC for various other metal ions at pH 6.

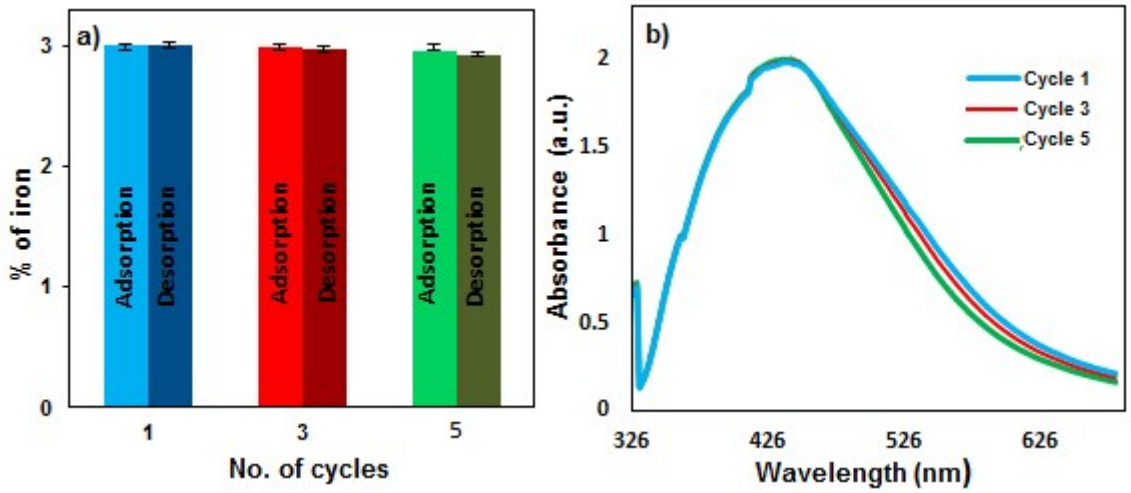

Figure S9: EDX elemental percentage of iron (a) and the UV-visible absorption spectra of P@MSMCs (b) after 1, 3 and 5 adsorption/desorption cycles. The error bars representing the standard error of three successive trials.