Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.

Supplementary Information

Optimization of Porous Structure of Superparamagnetic Nanoparticle Adsorbents for Higher and Faster Removal of Emerging Organic Contaminants and PAHs

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1. Analysis

Removal efficiency and sorption capacity of EOCs or PAHs was calculated as:

$$Removal\ efficiency = \frac{C_0 - C_t}{C_0} \times 100\% \quad (1)$$

$$Sorption\ capacity = q_e = \frac{(C_0 - C_t) \cdot V}{m} \quad (2)$$

where C_0 and C_t are the initial and final concentrations of EOCs (mg/L), m is the mass of Mag-PCMAs (g), and V is the volume of solution (L).

2. Properties of selected EOCs and PAHs

Table S1. Properties of selected EOCs and PAHs for Sorption Studies[1, 2]

	Compound name	Molecular mass (g/mol)	Octanol–water partition coefficient $logK_{ow}$	Initial Solution pH
EOCs	Methyl Orange	327.33	0.68	5.30
	Sulfamethoxazole	253.28	0.89	4.21
	Gemfibrozil	250.33	4.77	3.99
PAHs	Acenaphthene	154.21	3.92	4.97
	Phenanthrene	178.23	4.52	3.98

3. Mag-PCMAs characterization

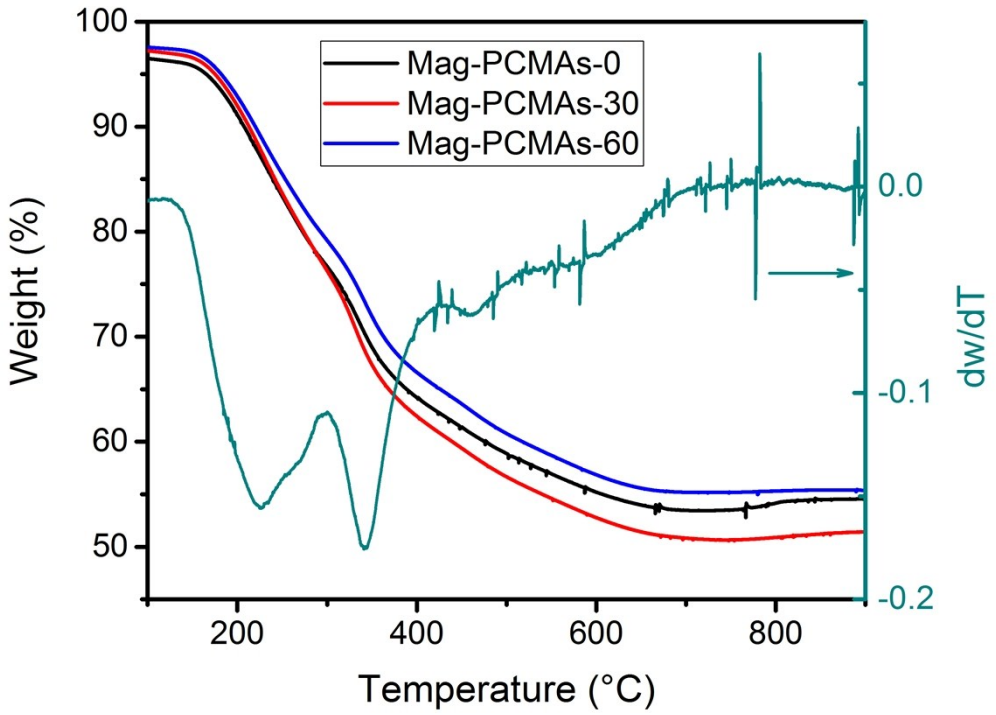

Figure S1. Thermogravimetric analysis (TGA) of Mag-PCMAs-0, Mag-PCMAs-30, and Mag-PCMAs-60

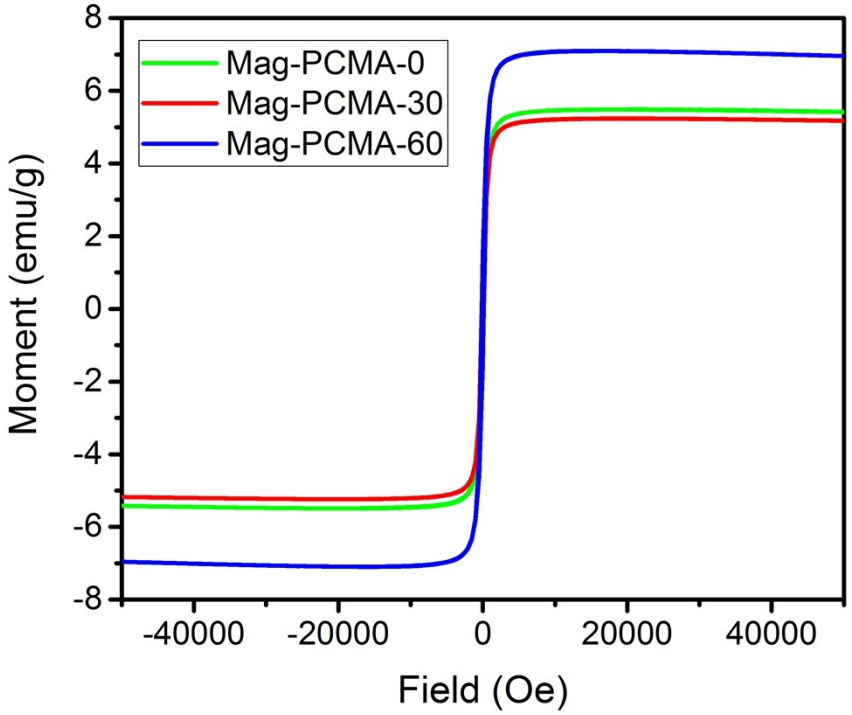

Figure S2. The magnetic hysteresis loops of Mag-PCMAs-0, Mag-PCMAs-30, and Mag-PCMAs-60.

4. Langmuir isotherm model

Table S2. Langmuir isotherm model parameters for EOCs and PAHs sorption on Mag-PCMAs

EOCs and PAHs	Mag-PCMAs	Langmuir		
		q_m (mg/g)	K_L (L/mg)	R^2
Sulfamethoxazole	Mag-PCMAs-0	87.4	0.72	0.996
	Mag-PCMAs-30	94.0	0.76	0.996
	Mag-PCMAs-60	113	0.75	0.996
Gemfibrozil	Mag-PCMAs-0	66.8	-0.02	0.929
	Mag-PCMAs-30	276	1.14	0.957
	Mag-PCMAs-60	465	0.04	0.981
Methyl Orange	Mag-PCMAs-0	177.	3.36	0.998
	Mag-PCMAs-30	185	-0.72	0.995
	Mag-PCMAs-60	444	0.21	0.908
Acenaphthene	Mag-PCMAs-0	0.48	-16.4	0.972
	Mag-PCMAs-30	0.56	-16.8	0.962
	Mag-PCMAs-60	1.46	-13.1	0.961
Phenanthrene	Mag-PCMAs-0	0.36	-20.1	0.967
	Mag-PCMAs-30	0.57	-14.5	0.922
	Mag-PCMAs-60	1.23	-32.0	0.920

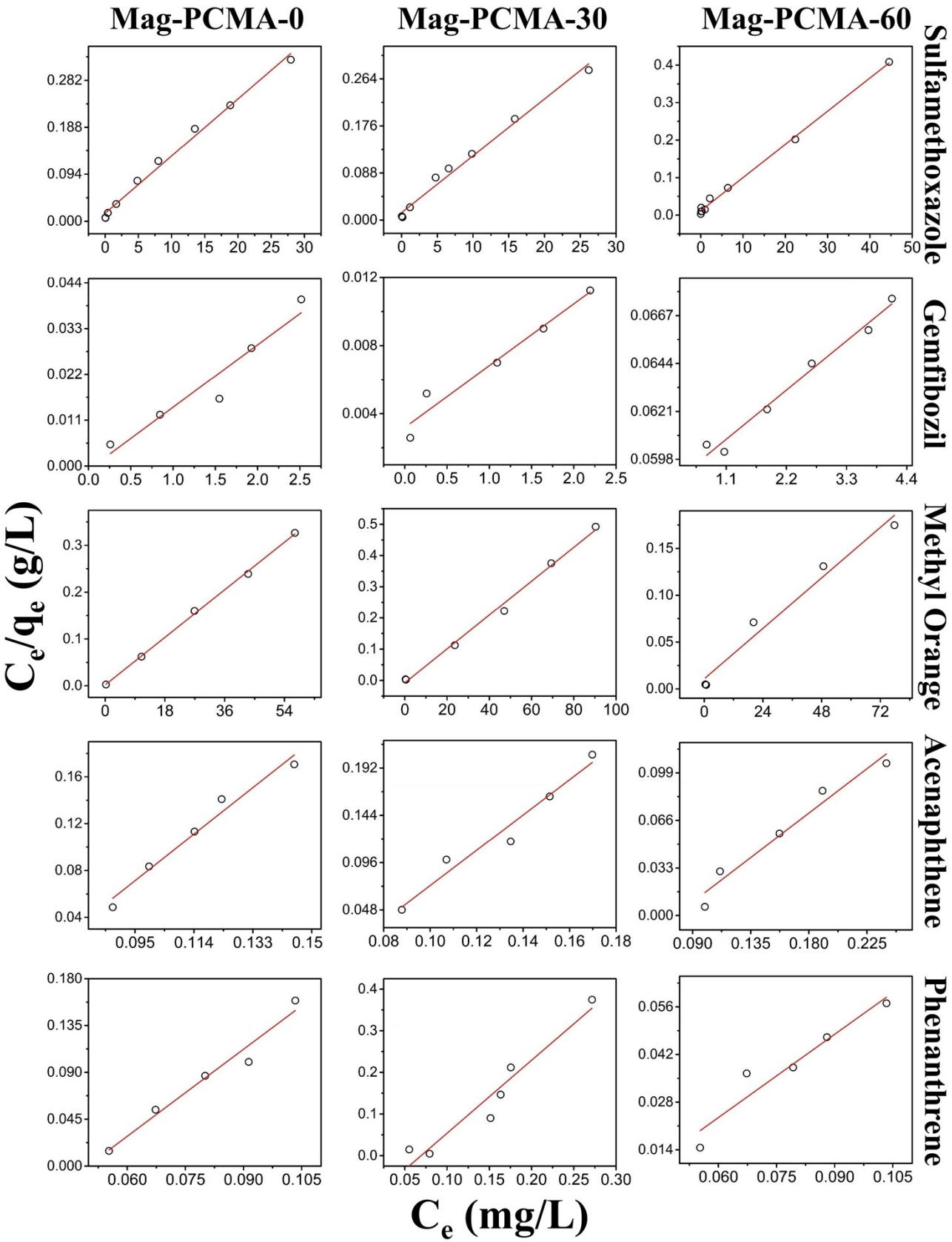
Mag-PCMA-0
Mag-PCMA-30
Mag-PCMA-60
Sulfamethoxazole
Gemfibozil
Methyl Orange
Acenaphthene
Phenanthrene
Ce/qe (g/L)
Ce (mg/L)

Figure S3. Adsorption of EOCs and PAHs (sulfamethoxazole, gemfibrozil, methyl orange, acenaphthene and phenanthrene) onto Mag-PCMA in solution with Langmuir adsorption isotherms fit, symbols represent experimental data, and red line represents model prediction.

References:

1. Huang, Y. X.; Keller, A. A. Magnetic Nanoparticle Adsorbents for Emerging Organic Contaminants. *Acs Sustain Chem Eng* 2013, 1, 731-736.
2. Watts, R. J. *Hazardous wastes: sources, pathways, receptors*. 1998.