

Supporting Information

Effective and simple removal of Hg from real waters by robust bio-nanocomposite.

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Tables

Table SI-1. Elemental analysis of the bottled water matrix (Fastio®) used in the study

Bottled water (Fastio®) Initial pH = 6.2			
<i>Major elements</i> (mg L ⁻¹)		<i>Minor elements</i> (µg L ⁻¹)	
Ca	1.3	B	20
Na	4.1	Al	50
K	0.6	Cr	1.3
Mg	0.7	Fe	61
P	0.4	Co	< 1
Si	0.8	Ni	< 1
Cl	4.2	Cu	3.1
		Zn	20
		As	< 2
		Se	< 1
		Sr	6.3
		Cd	<0.1
		Sb	< 0.1
		Ba	3.1
		Pb	< 0.1

Table SI-2 gathers the mathematical equations used in the kinetic modelling of the sorption data. q_t is the amount of metal sorbed per gram of sorbent at given time t (µg g⁻¹), q_e amount of metal adsorbed per gram of materials at equilibrium (µg g⁻¹), k_1 is the

rate constant of pseudo-first order (h^{-1}), k_2 rate constant of pseudo-second order ($\text{g } \mu\text{g}^{-1} \text{h}^{-1}$), α initial sorption rate ($\mu\text{g g}^{-1} \text{h}^{-1}$), β desorption constant ($\text{g } \mu\text{g}^{-1}$).

Table SI-2. Sorption reaction kinetic models and corresponding mathematical equations used in the study.

Kinetic model	Equation	References
Pseudo-first-order (Lagergren)	$q_t = q_e (1 - e^{-k_1 t})$	1
Adsorption capacity Pseudo-second-order (Ho)	$q_t = \frac{q_e^2 k_2 t}{1 + q_e k_2 t}$	2
Elovich	$q_t = \frac{1}{\beta} \ln(1 + \alpha \beta t)$	3

Boyd's film-diffusion ⁴ and Webber's pore-diffusion ⁵ were applied to study the diffusion mechanism and which rate-controlling step drives the process.

The film-diffusion model presented by Boyd states that the main opposition to diffusion is in the boundary layer surrounding the sorbent particle ^{6,7}, expressed as:

$$F = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \left(\frac{1}{n^2} \right) \exp(-n^2 Bt) \quad (4)$$

where F is the fractional attainment of equilibrium, at different times, t , and Bt is a function of F :

$$F = \frac{q_t}{q_e} \quad (5)$$

Bt can be calculated as:

$$\text{For } F \text{ values} > 0.85 \quad Bt = -0.4977 - \ln(1 - F) \quad (6)$$

$$\text{For } F \text{ values} < 0.85 \quad Bt = \left(\sqrt{\pi} - \sqrt{\pi - \frac{\pi^2 F}{3}} \right)^2 \quad (7)$$

If the Boyd's plot (Bt vs t) excludes the origin, the film diffusion or chemical reaction must be the rate-controlling step, whereas if the plot is linear and passes through the origin, it is the intraparticle-diffusion that mostly controls the rate of mass transfer.

Weber's intraparticle-diffusion model is defined by the equation ^{6,7} :

$$q_t = k_i t^{1/2} \quad (8)$$

in which k_i is the intraparticle-diffusion parameter ($\text{mg g}^{-1} \text{h}^{1/2}$). If a plot of qt vs t is a straight line with a slope that equals k_i and an intercept equal to zero, the intraparticle-diffusion must be the rate-limiting step. If not, there must be another mechanism along with intraparticle diffusion must be considered. To analyse the experimental data under the film-diffusion and the intraparticle-diffusion models, and to predict the corresponding diffusion coefficients, a piecewise linear regression methodology (PLR), proposed by Malash et al. ⁶, was performed using a Microsoft® Excel™ worksheet developed by these authors.

Figures

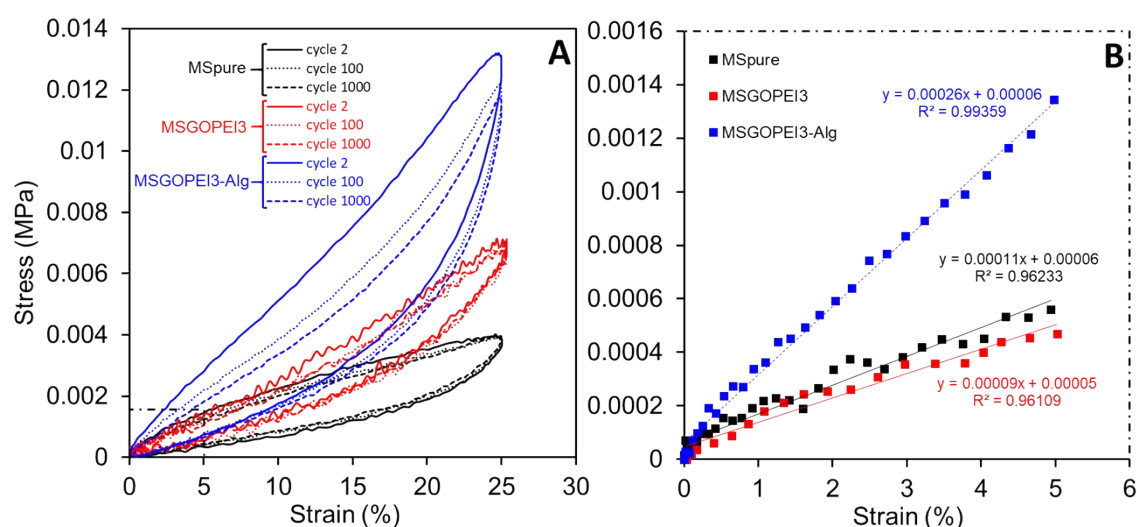


Fig. S1 – A) wet cyclic compression mechanical test (25 % strain) up to 1000 cycles, B) inset on the initial linear part of the plot for the calculation of Young Modulus.

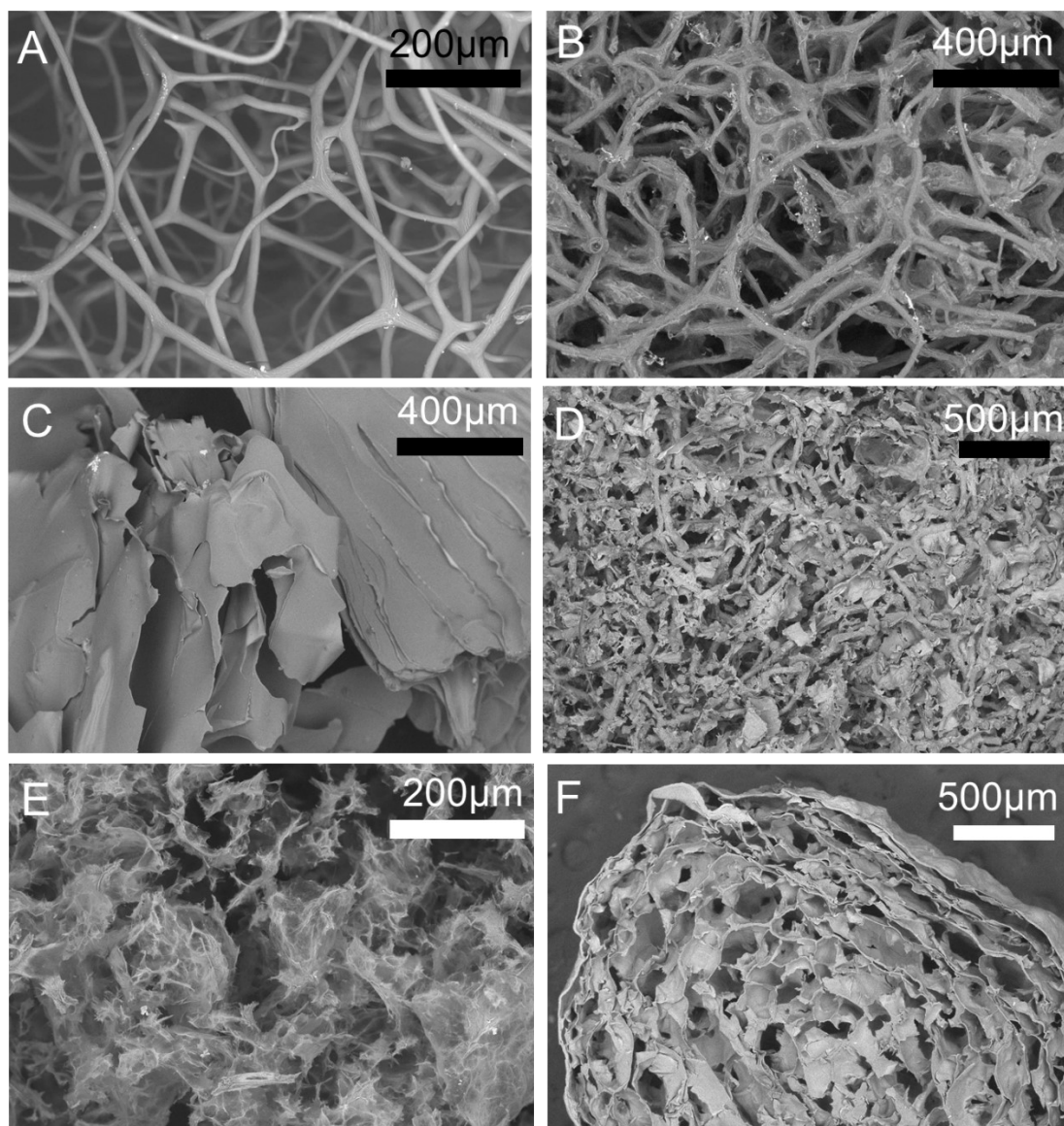


Fig. S2 – SEM micrographs of the several samples studied in this work. A) MS, B) MSGOPEI3, C) Alg, D) MSGOPEI3-Alg, E) GOPEI and F) GOPEI-Alg.

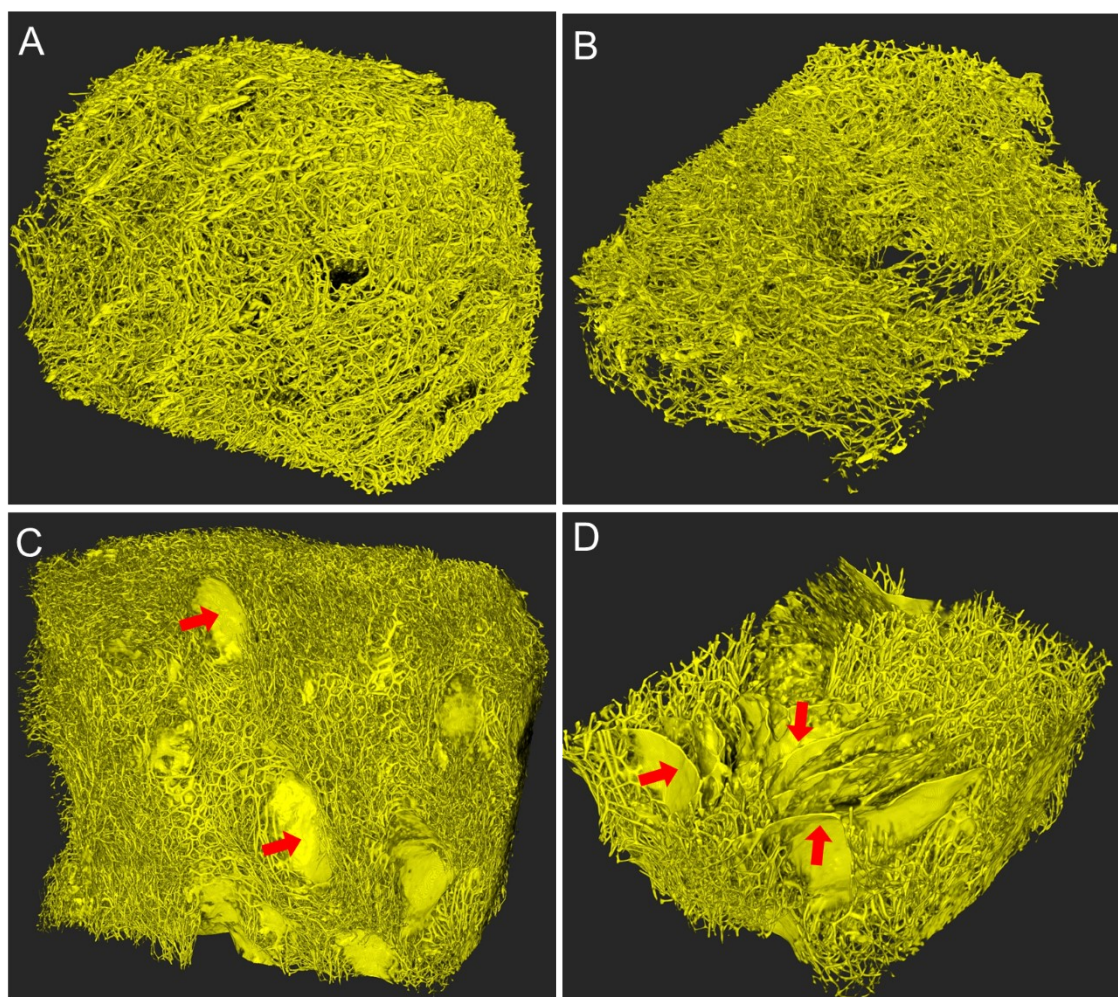


Fig. S3 – CT scan of A) MS sample, B) digital cross-section of MS, C) MSGOPEI3-Alg and D) digital cross-section of MSGOPEI3-Alg. This technique allowed to verify of the distribution of GOPEI-Alg layers (pointed out with the red arrows) throughout the entire volume of the MSGOPEI3 dices.

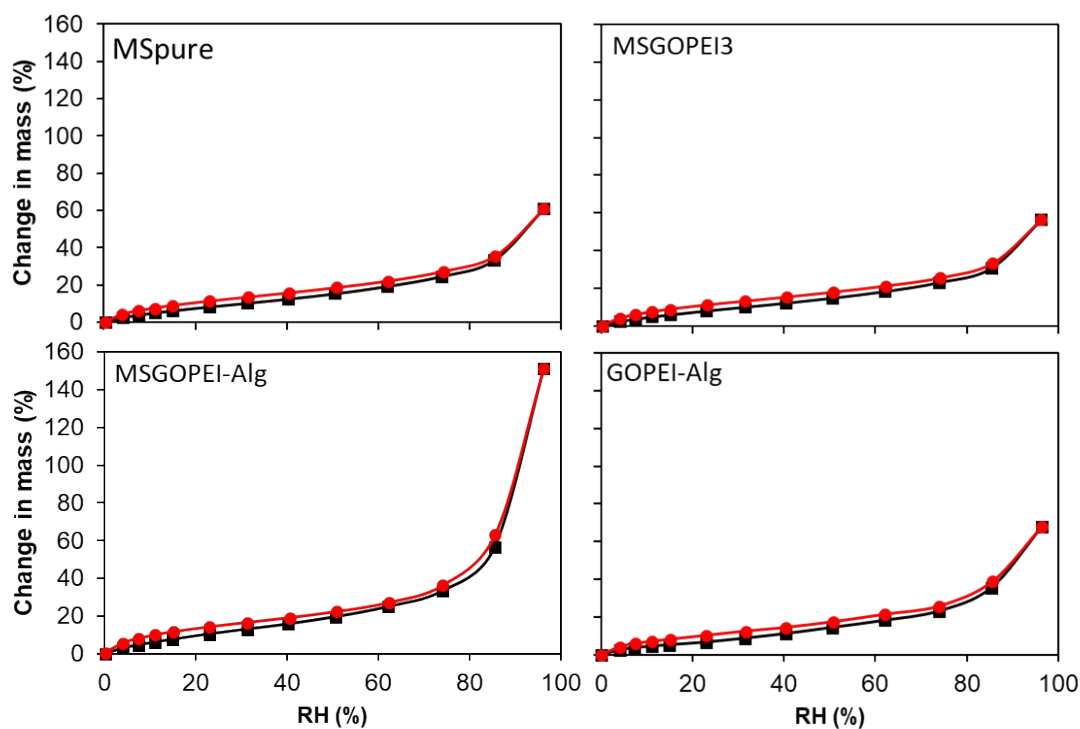


Fig. S4 – Water vapor sorption isotherms for the several samples studied.

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