## **Evaluation of Polyurea-Crosslinked Alginate Aerogels for Seawater Decontamination**

Patrina Paraskevopoulou <sup>1,\*</sup>, Grigorios Raptopoulos <sup>1</sup>, Faidra Leontaridou <sup>1</sup>, Maria Papastergiou <sup>1</sup>, Aikaterini Sakellari <sup>2</sup> and Sotirios Karavoltsos <sup>2,\*</sup>

## Table of contents

Figure S1. Optical photograph and size distribution of X-Ca-alginate aerogel beads (diameters measured with	
ImageJ; histogram calculated using OriginPro 9.0). Mean diameter and sample size (N) are shown on the Figure	. 2
Figure S2. ATR-FTIR spectra of X-Ca-alginate aerogel beads, as indicated. The characteristic peaks for the Ca-	
alginate skeleton are noted with blue and the ones for polyurea (PUA) are noted with purple	. 2
Figure S3. <sup>13</sup> C CPMAS NMR spectra of X-Ca-alginate aerogel beads	.3
Figure S4. N <sub>2</sub> -sorption diagram of crosslinked X-Ca-alginate aerogel beads. Inset shows pore size distribution by	
the BJH method	. 3
Figure S5. Pb <sup>II</sup> uptake from ultrapure water solutions by X-Ca-alginate aerogel beads versus time. Initial Pb <sup>II</sup>	
concentrations: 0.01 (A), 0.1 (B) and 1 (C) mg L <sup>-1</sup>	.4
$\label{eq:Figure S6.} Freundlich \ isotherm \ for \ Pb^{II} \ up take \ from \ ultrapure \ water \ solutions \ by \ X-Ca-alginate \ aerogel \ beads. \ Q_{eq}$	:
$Pb^{II}$ uptake at equilibrium. $C_{eq}$ : concentration of $Pb^{II}$ in the solution at equilibrium.	.4

Table S1. Selected material properties of X-Ca-alginate aerogel beads......5

<sup>&</sup>lt;sup>1</sup> Inorganic Chemistry Laboratory, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, 15771 Athens, Greece; <u>grigorisrap@chem.uoa.gr</u> (G.R.); <u>faidraleo@chem.uoa.gr</u> (F.L.); <u>mapapast@chem.uoa.gr</u> (M.P.)

<sup>&</sup>lt;sup>2</sup> Laboratory of Environmental Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, 15784 Athens, Greece; <u>esakel@chem.uoa.gr</u> (A.S.)

<sup>\*</sup> Correspondence: paraskevopoulou@chem.uoa.gr; Tel.: +30-210-727-4381(P.P.); skarav@chem.uoa.gr; Tel.: +30-210-727-4269 (S.K.)



**Figure S1.** Optical photograph and size distribution of X-Ca-alginate aerogel beads (diameters measured with ImageJ; histogram calculated using OriginPro 9.0). Mean diameter and sample size (N) are shown on the Figure.



**Figure S2.** ATR-FTIR spectra of X-Ca-alginate aerogel beads, as indicated. The characteristic peaks for the Ca-alginate skeleton are noted with blue and the ones for polyurea (PUA) are noted with purple.



Figure S3. <sup>13</sup>C CPMAS NMR spectra of X-Ca-alginate aerogel beads.



**Figure S4.** N<sub>2</sub>-sorption diagram of crosslinked X-Ca-alginate aerogel beads. Inset shows pore size distribution by the BJH method.



**Figure S5.** Pb<sup>II</sup> uptake from ultrapure water solutions by X-Ca-alginate aerogel beads versus time. Initial Pb<sup>II</sup> concentrations: 0.01 (A), 0.1 (B) and 1 (C) mg L<sup>-1</sup>.



**Figure S6.** Freundlich isotherm for Pb<sup>II</sup> uptake from ultrapure water solutions by X-Ca-alginate aerogel beads.  $Q_{eq}$ : Pb<sup>II</sup> uptake at equilibrium.  $C_{eq}$ : concentration of Pb<sup>II</sup> in the solution at equilibrium.

Table S1. Selected material properties of X-Ca-alginate aerogel beads.

Sample ª	Bulk density ρ <sub>b</sub> (g cm <sup>-3</sup> )	Skeletal density ₽s (g cm <sup>-3</sup> )	Porosity ⁵ ∏(% v/v)	BET surf. area σ(m² g <sup>-1</sup> ) [micropore surf. area] °	V <sub>Total</sub> d (V <sub>1.7-300nm</sub> ) e (cm <sup>3</sup> g <sup>-1</sup> )	Av. pore diam. <sup>f</sup> (4V <sub>Total</sub> /σ) (nm)	Particle radius <sup>g</sup> <i>r</i> (nm)
X-Ca-alginate aerogel beads	0.150±0.009	1.485±0.005	90	459 [28]	6.0 (2.9)	25 (50)	4.4 (4.7)

<sup>a</sup> The concentration of the sodium alginate solution was 3% w/w. <sup>b</sup> Porosity calculated according to the formula:  $(\rho_{s-}-\rho_{o})/\rho_{s}$ , where  $\rho_{s}$ : skeletal density and  $\rho_{o}$ : bulk density. <sup>c</sup> Micropore surface area *via t*-plot analysis, according to the Harkins and Jura model. <sup>d</sup> Total pore volume calculated according to formula:  $1/\rho_{o-}-1/\rho_{s}$ . <sup>e</sup> Cumulative volume of pores between 1.7 and 300 nm from N<sub>2</sub>-sorption data and the BJH desorption method. <sup>f</sup> Calculated by the 4 *V*/ $\sigma$  method; *V* was set equal to the maximum volume of N<sub>2</sub> adsorbed along the isotherm as  $P/P_{o} \rightarrow 1.0$ . For the number in parentheses, *V* was set equal to *V*<sub>Total</sub> from the previous column. <sup>g</sup> Particle radius calculated by the formula:  $r = 3/(\rho_{s} \times \sigma)$ , where  $\sigma$ : BET surface area. For the number in parentheses,  $\sigma$  was set equal to the external surface area,  $\sigma_{ext}$ , calculated from the BET surface area minus the micropore surface area.