Supplementary information

Development of sulfonated polystyrene resin-supported tungsten oxide for Pb^{2+} ion sequestration

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Fig. S1. Digital photographs of PS (a), PSWO (b), SO_3-PS (c) and SO_3-PSWO (d).

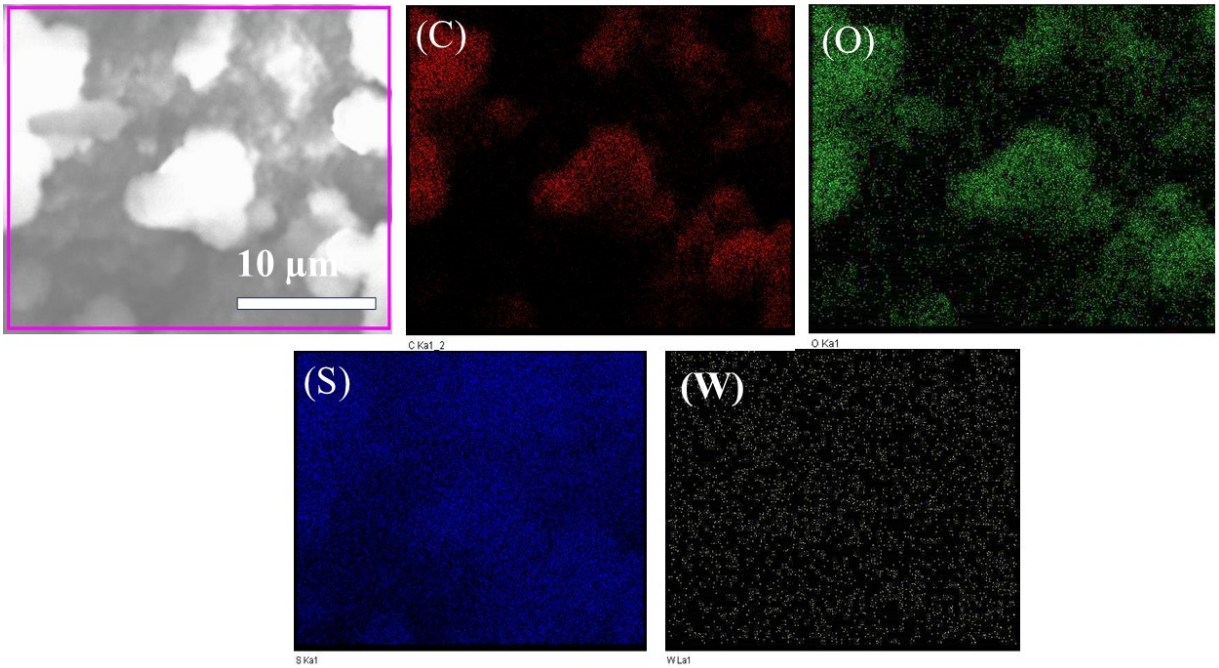

Fig. S2. Elemental dot mapping of SO_3-PSWO.

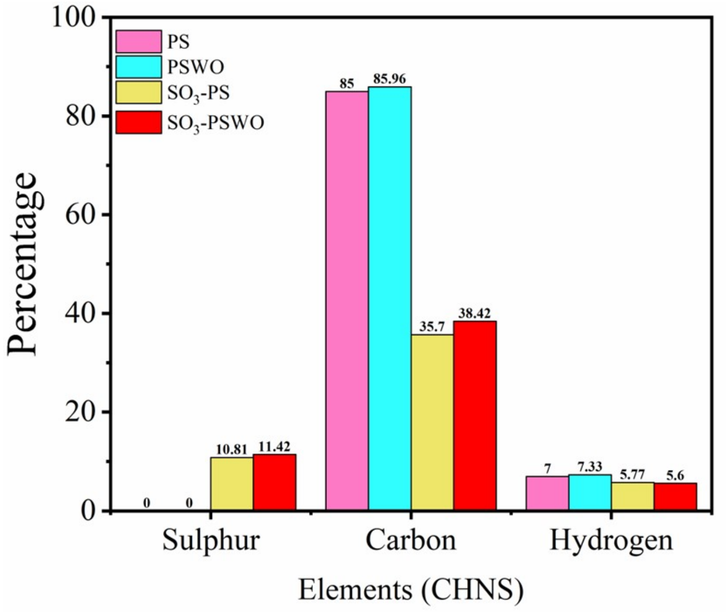

Fig. S3. C, H, and S concentration in prepared samples determined through CHNS analysis.

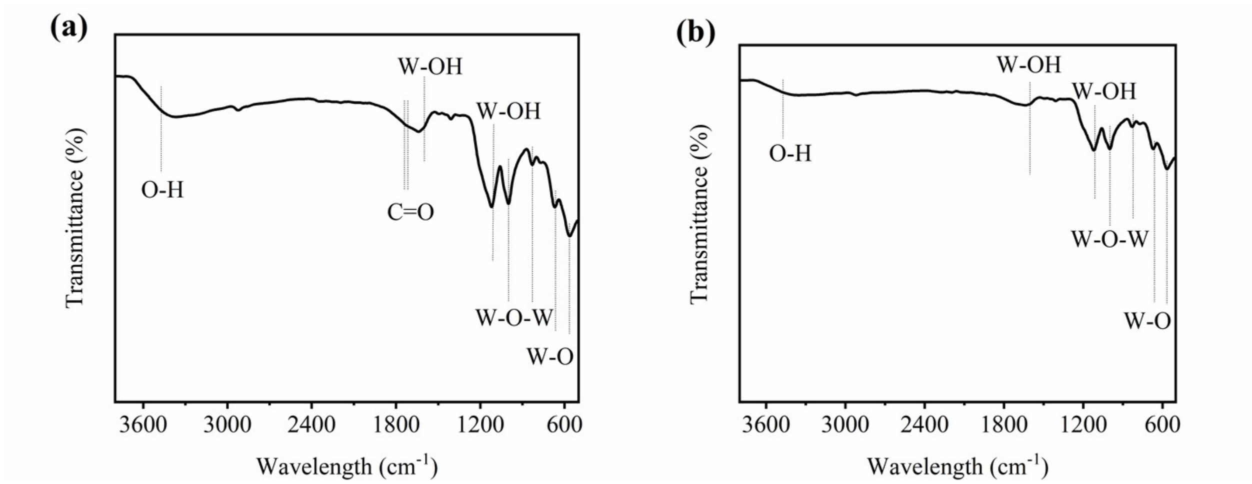

Fig. S4. FTIR Spectra of SO_3-PSWO (a) before adsorption of Pb^{2+} (b) after adsorption of Pb^{2+}

The FTIR spectra of SO_3-PSWO before adsorption (Fig. S4a) confirm the successful loading of tungsten. After adsorption, the decrease in peak intensity (Fig. S4b) indicates the adherence of Pb^{2+} ions onto the SO_3-PSWO surface.

Before adsorption (Fig. S4a), a broad band between 3800–3000 cm^{-1} is observed in SO_3-PSWO, attributed to the stretching vibrations of O–H groups in both surface W–OH and adsorbed water. This suggests the presence of tungsten oxide in the host resin[1]. However, after adsorption (Fig. S4b), this band decreases significantly, almost disappearing, likely due to Pb^{2+} ions interacting with SO_3-PSWO and occupying the adsorption sites.

A peak at 1728–1740 cm^{-1} corresponds to the stretching vibrations of the C=O group, indicating the retention of some residual acetyl groups within the polymer matrix. This aligns with literature values for C=O stretching in lignocellulosic materials and cellulose acetylation[2],[3]. After adsorption, the peak at 1728–1740 cm^{-1} nearly vanishes.

At 1605 cm^{-1}, a prominent peak represents the symmetric stretching vibrations associated with WO_3 and interlinked water molecules (W–OH, H_2O)[4],[5]. After Pb^{2+} adsorption, interactions with W–OH groups alter their vibrational bands, leading to a decrease in peak intensity, as shown in Fig. S4b.

Another peak around 1100 cm⁻¹ in SO_3-PSWO corresponds to the bending vibrations of W–OH[6]. A similar peak has been reported in the work of Kustova et al. (2011), confirming this spectral range[7]. Following Pb^{2+} adsorption, the intensity decreases as the ions bind to O–H groups in tungsten oxide, reducing the number of free-bending vibrations.

In the 1000–500 cm⁻¹ range, multiple bands appear in SO_3-PSWO, attributed to vibrational modes of W–O–W, O–W–O, W–O, W–OH, and W=O bonds[6],[8]. These bands also decrease in intensity after Pb^{2+} adsorption, suggesting chemical interactions between Pb^{2+} ions and the active sites (e.g., W–OH groups) on the resin surface. The observed reduction in peak intensity is likely due to the formation of chemical bonds between Pb^{2+} ions and these functional groups, which restrict their characteristic vibrational modes.

Thus, the surface coverage of SO_3-PSWO by Pb^{2+} ions and their interaction with functional groups during the adsorption process likely contribute to the observed decrease in peak intensity. This reduction is further supported by findings from H. Joga Rao (2020) [9].

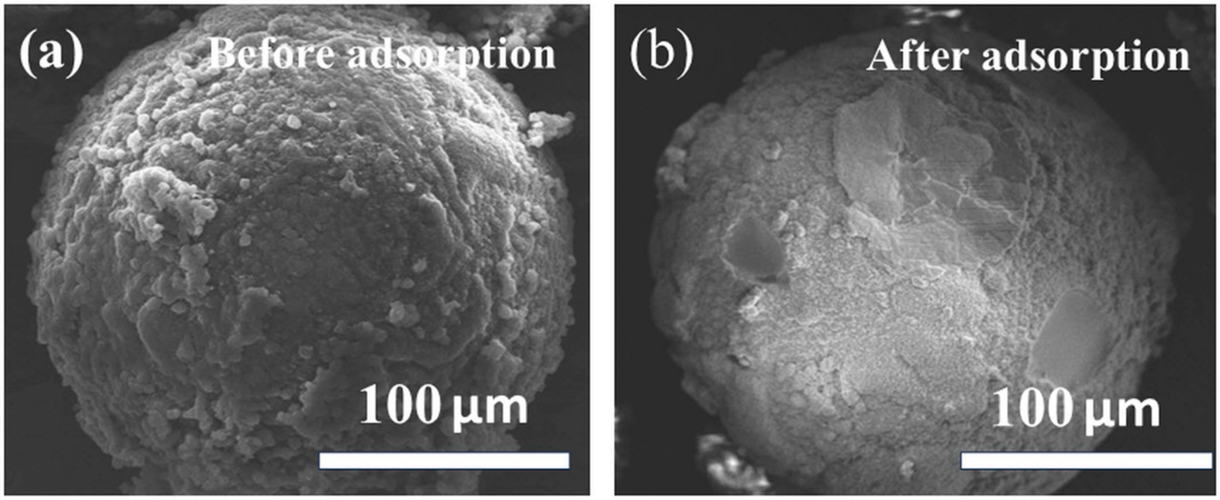

Fig. S5. SEM images of SO_3-PSWO before adsorption of Pb^{2+} (a) and after adsorption of Pb^{2+} (b).

Reference

1. S. M. Kanan and C. P. Tripp, Curr. Opin. Solid State Mater. Sci*,* 2007, **11**, 19-27.
2. B. MOHEBI, J. Agric. Sci. Technol, 2008, 10: 253-259.

3. M. O. Adebajo and R. L. Frost, Spectrochim. Acta A Mol. Biomol. Spectrosc*,* 2004, **60**, 2315-2321.

4. V. B. Kumar and D. Mohanta, Bull. Mater. Sci*,* 2011, **34**, 435-442.

5. T. Muzaffar, R. Y. Khosa, U. Iftikhar, R. M. Obodo, S. Sajjad and M. Usman, J. Clust. Sci*,* 2021, 1-10.

6. R. Hatel and M. Baitoul, Mater. Chem. Phys*,* 2019, **225**, 169-173.

7. G. Kustova, Y. A. Chesalov, L. Plyasova and A. Nizovskii, Vib. Spectrosc., 2011, **55**, 235-240.

8. S. Bai, Y. Ma, R. Luo, A. Chen and D. Li, *RSC Adv,* 2016, **6**, 2687-2694.

9. H. J. Rao, Nat. Environ. Pollut. Technol*,* 2021, **20**.