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## Title

### ***Removal of Mo(VI), Pb(II), and Cu(II) from wastewater using electrospun cellulose acetate/chitosan biopolymer fibers***

## Abstract

Environmentally friendly polymers such as cellulose acetate (CA) and chitosan (CS) were used to obtain electrospun fibers for Cu<sup>2+</sup>, Pb<sup>2+</sup>, and Mo<sup>6+</sup> capture. The solvents dichloromethane (DCM) and dimethylformamide (DMF) allowed the development of a surface area of 148 m<sup>2</sup> g<sup>-1</sup> for CA fibers and 113 m<sup>2</sup> g<sup>-1</sup> for cellulose acetate/chitosan (CA/CS) fibers. The fibers were characterized by IR-DRIFT, SEM, TEM, CO<sub>2</sub> sorption isotherms at 273 K, Hg porosimetry, TGA, stress-strain tests, and XPS. The CA/CS fibers had a higher adsorption capacity than CA fibers without affecting their physicochemical properties. The capture capacity reached 102 mg g<sup>-1</sup> for Cu<sup>2+</sup>, 49.3 mg g<sup>-1</sup> for Pb<sup>2+</sup>, and 13.1 mg g<sup>-1</sup> for Mo<sup>6+</sup>. Furthermore, optimal pH, adsorption times  $q_t$ , and C<sub>0</sub> were studied for the evaluation of kinetic models and adsorption isotherms. Finally, a proposal for adsorbate-adsorbent interactions is presented as a possible capture mechanism where, in the case of Mo<sup>6+</sup>, a computational study is presented. The results demonstrate the potential to evaluate the fibers in tailings wastewater from copper mining. © 2024 Elsevier B.V.

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functional theory; diffuse reflectance infrared Fourier transform spectroscopy; energy dispersive X ray spectroscopy; gas chromatography; heavy metal removal; histogram; inductively coupled plasma atomic emission spectrometry; isotherm; kinetics; light microscopy; mathematical model; mining; nonhuman; pH; physical chemistry; porosimetry; procedures; scanning electron microscopy; stress strain test; tensile strength; thermogravimetry; transmission electron microscopy; wastewater; X ray diffraction; Young modulus; chemistry; isolation and purification; water management; water pollutant; Metal ions

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carbon dioxide, 124-38-9, 58561-67-4; cellulose acetate, 9004-35-7; chitosan, 9012-76-4; copper, 15158-11-9, 7440-50-8; dichloromethane, 75-09-2; lead, 7439-92-1, 13966-28-4; molybdenum, 7439-98-7; n,n dimethylformamide, 68-12-2; cellulose, 61991-22-8, 68073-05-2, 9004-34-6; acetylcellulose, ; Biopolymers, ; Cellulose, ; Chitosan, ; Copper, ; Lead, ; Wastewater, ; Water Pollutants, Chemical,

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Autosorb iQ XR 2, Quantachrome; JEM 1400 Plus transmission electron microscope, Jeol; Merlin VP scanning electron microscope, Carl Zeiss; Quantax 400 energy dispersive X ray microanalysis system, Bruker; SDT 2980, TA Instruments; SupraSolv gas chromatograph, Sigma Aldrich; TL 01 electrospinning machine, Tong li tech; iCE 3000, Thermo

## **Manufacturers**

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