Supplementary material

A green L-cysteine modified cellulose nanocrystals biosorbent for adsorption of mercury ions from aqueous solutions

Weixue Li, Benzhi Ju *, Shufen Zhang

State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian 116024, PR China

Corresponding authors. Tel.: +86 411 84986269; fax: +86 411 84986264.

E-mail: jubenzhi@dlut.edu.cn (B. Ju).

Experimental

Characterization

Fourier transform infrared spectroscopy (FT-IR)

FT-IR spectra of samples were recorded over the range 4000 to 400 cm^{-1} on a Thermo Scientific Nicolet 6700 FT-IR spectrometer (ThermoFisher Scientific, Waltham, MA, USA).

X-ray photoelectron spectroscopy (XPS)

X-ray photoelectron spectroscopy (XPS) was performed to determine the surface compositions of the samples with a Thermo Scientific 250Xi spectrometer (Thermo Fisher Scientific).

^{13}C CP-MAS solid-state NMR

Solid-state NMR experiments were performed with an Agilent DD2 500 MHz (B0=11.7T) spectrometer operating, using the combination of cross-polarization, high-power proton decoupling and magic angle spinning (CP/MAS) method.

Zeta potential

The zeta potential was measured using a Zetasizer NanoZS-90 (Malvern Instruments, Ltd., Malvern, Worcs., UK) at 25 °C, 0.01 M KCl.

Scanning electron microscopy (SEM)

The morphology of CNCs, DAC nanocrystals and Lcys-CNCs was analyzed by scanning electron microscopy (SEM), on a Hitachi FESEM SU8220 system (Hitachi Corp., Tokyo, Japan). Energy dispersive X-ray (EDX) spectroscopy was conducted using an EDX analyzer (Horiba Ltd., Kyoto, Japan).

Inductively coupled plasma mass spectrometry (ICP-MS)

ICP-MS using a PerkinElmer Nex ION 300D ICP-mass spectrometer (PerkinElmer, Waltham, MA, USA).

Specific surface area measurement

The surface area according to the Brunauer, Emmett and Teller (BET) algorithm surface area was determined by measuring nitrogen adsorption on an Autosorb-iQ-C gas sorption analyzer (Quantachrome Instruments, Boynton Beach, FL, USA).

Elemental analysis

Elemental analysis was conducted on an Elementar Vario EL CUBE elemental

analyzer (Elementar Analysensysteme GmbH, Hanau, Germany).

Results and discussion

Table S1 Table of XPS data for Lcys-CNCs

Orbital	Component	Binding Energy (eV)	Relative (%)
C 1s	-C-C	283.8	40.8
	-C-O	284.7	39.0
	-O-C-O	286.0	9.5
	-O-C=O	286.8	10.6
O 1s	-C-O-H	530.0	17.4
	-O-C-O, -C=O	531.1	82.6
S 2p	-SH (j = 3/2)	161.6	66.5
	-SH (j = 1/2)	162.8	33.4
	$-SO_3^-$ (j = 3/2)	167.0	67.1
	$-SO_3^-$ (j = 1/2)	168.4	32.9
N 1s	-NH-	397.8	78.6
	$-N^+H_2-$	400.1	21.4

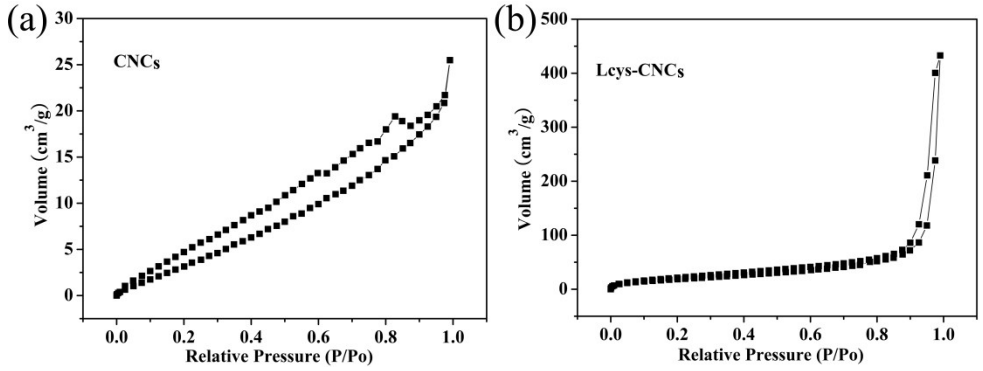

Fig. S1 N_2 adsorption-desorption isotherms of CNCs (a) and Lcys-CNCs (b).

Table S2 Length and width of Lcsy-CNCs and Hg(II)-loaded Lcsy-CNCs

	Width (nm)	Length (nm)
Lcsy-CNCs	25±6	228±57
Hg(II)-loaded Lcsy-CNCs	35±11	-

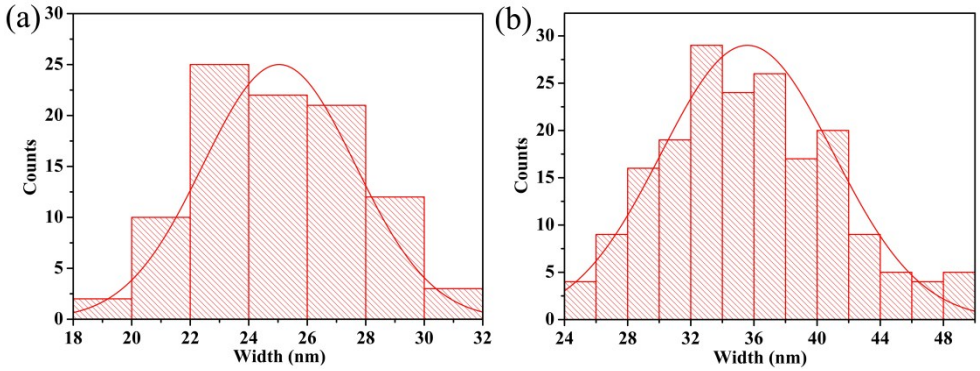

Fig. S2 Width distribution from SEM of Lcsy-CNCs (a) and Hg(II)-loaded Lcsy-CNCs (b).