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Electrospun Chitosan-Polyvinyl alcohol composite nanofibers loaded with Cerium for efficient removal of Arsenic from contaminated water

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Figure S1 shows the elemental (C, O, Ce and As) mapping of Ce- CHT/PVA composite nanofibers after As (III) adsorption, it shows the uniform distribution of all elements throughout the nanofibers sheet.

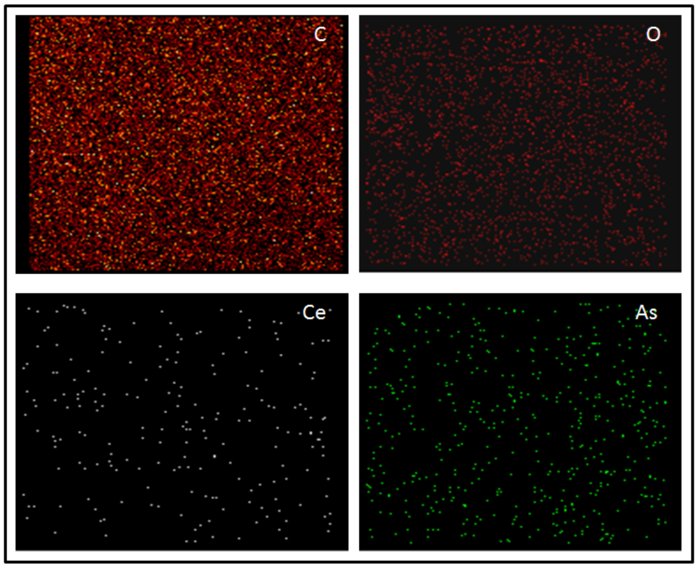

Figure S1: Elemental (C, O, Ce As) mapping of Ce-CHT/PVA composite nanofibers after As (III) adsorption

Figure S2 shows the effect of temperature on As (III) adsorption and reveals that material shows high adsorption between 20-35°C. The effect of temperature on As (III) adsorption has been studied at varying temperature (10-65°C) at optimized pH. The low temperature obtained by cooling test solution in ice bath, while high temperature obtained by heating on magnetic stirrer.

The maximum adsorption observed as shown in (supplementary information as Fig.S2) between temperatures 20-35°C. While on increasing temperature (>35 °C) or decreasing (<20 °C), As (III) adsorption decreases This can be due to the fact that rise in temperature would increase the number of active sites on the surface of composite nanofibers and may enhance the rate of protonation of -NH_2 group. But further on decreasing or increasing temperature, the protonation of -NH_2 group remains unaffected probably due to the surface complexes and interactions.

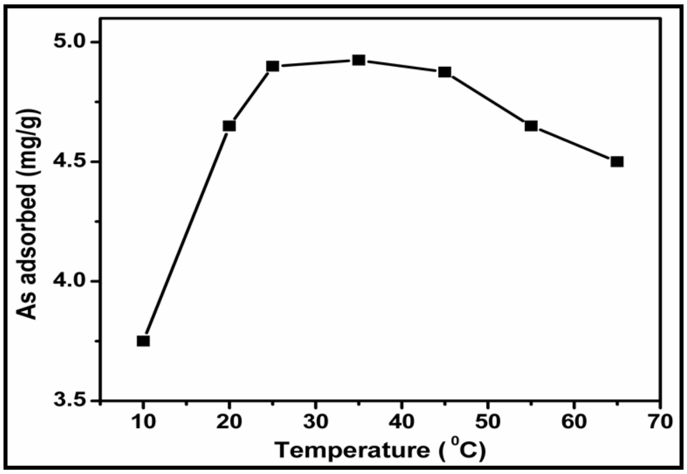

Figure S2 : Effect of temperature on As adsorption

Figure S3 shows, FTIR spectra of CHT/PVA, Ce-CHT/PVA and Ce-CHT/PVA composite nanofibers with As (III). The curve (a), denotes the spectra of CHT/PVA nanofibers, having adsorption band at around 3342 cm^{-1} is due to the -OH stretching that superimposes with the-NH bands of amine and amide of chitosan. The absorption peak at 1724 cm^{-1} is due to the presence of C=O-NH group in CHT/PVA nanofiber. The absorption peaks at 1635 cm^{-1}, 1589 cm^{-1} and 1363cm^{-1} are due to amide (I, II, III) vibrations, which are considered as characteristics peaks of chitosan. The adsorption peak at 1079 cm^{-1} and 1421 cm^{-1} are due C=O stretching vibration and-OH stretching of PVA respectively. The peak at 2927 cm^{-1} is for CHT/PVAbut on Ce functionalization, the intensity of peak decreases which minor shift to 2923 cm^{-1} and after As (III) adsorption the peak appears at 2937 cm^{-1}. All these peaks (2927 cm^{-1}, 2923 cm^{-1} and 2937 cm^{-1}) are due to the presence of symmetric C-H stretching vibrations in curve ‘a’, ‘b’ and ‘c’ respectively. In case Ce- CHT/PVA composite nanofibers (Fig. S3 curve(b)), adsorption peaks at 1363 cm^{-1} and 1075 cm^{-1} in curve (a), shifted towards higher wave number 1371 cm^{-1} and

1095 cm^{-1} (curve b) may be due to -NH group from chitosan that interacts with cerium (III) in Ce- CHT/PVA. After absorption of As (III) on Ce-CHT/PVA nanofibers (curve c, Figure S3), it is observed that after interaction of As (III) with -NH$_2$ (1643cm^{-1}, 1579 cm^{-1}) and Ce (1376cm$^{-1,}$ 1095 cm^{-1}), the intensity of these peaks increases. The some peak positions are shifted to higher wave number due to the adsorption of As (III) on the composite nanofibers surface.

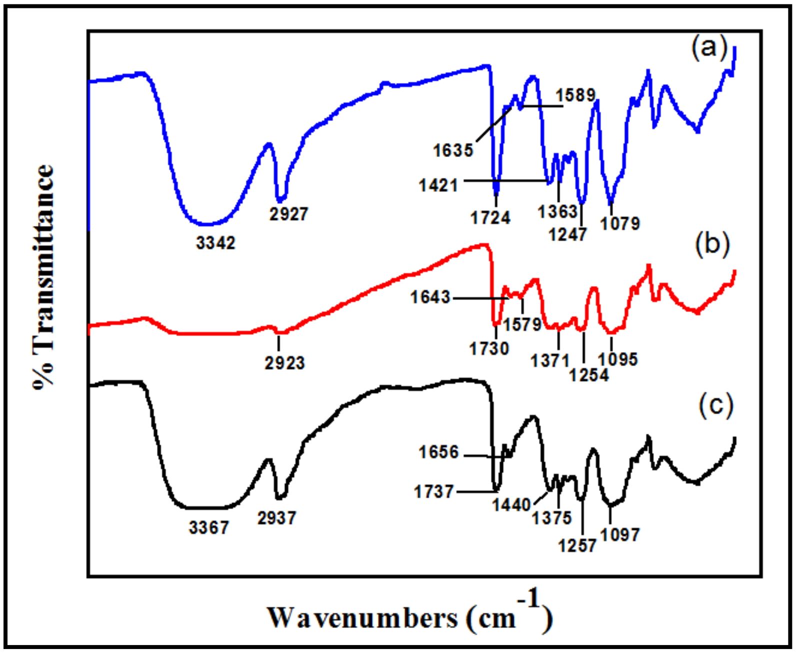

Figure S3: FTIR spectra of (a) PVA/CHT, (b) Ce-CHT/PVA and (c) Ce-CHT/PVA after adsorption of As (III)

The XRD spectra of Ce-CHT/PVA before and after As (III) adsorption is given in (Supplementary information as Fig. S4) reveals that peaks around at 2θ=10.7 and 20.4^{0} is of PVA. Appearance of two peaks at 10.5^{0} and 20.1^{0} are contributions of CHT nanofibers which is due to string inter and intra molecular hydrogen bonding in CHT. In the Ce-CHT/PVA composite nanofibers curve ‘a’), the peaks at 2θ= 9.16^{0} and 19.32^{0} are possibly due to the interaction of PVA and CHT while some other peaks at 38^{0} and 45^{0} may be due to the Ce (III) complexation with CHT/PVA. The literature reveals that peaks around 34^{o} and 37^{o}are due the Ceria structure. In the present work, peaks are observed around at 38^{o} and 45^{o} which may be due the interaction of cerium with CHT/PVA resulting in formation of unknown crystallite phases. However, after adsorption of As (III) on composite nanofibers the peaks at 9.16 and 19.32^{o} in (Fig.S4, curve a) are shifted to 2θ= 9.3° and 19.86° (**curve ‘b’, Fig.S4**). The shifting and increases in peak intensity confirms the presence of As (III) adsorption on Ce-CHT/ PVA composite nanofibers. These results are in agreement with observation of SEM and FTIR.

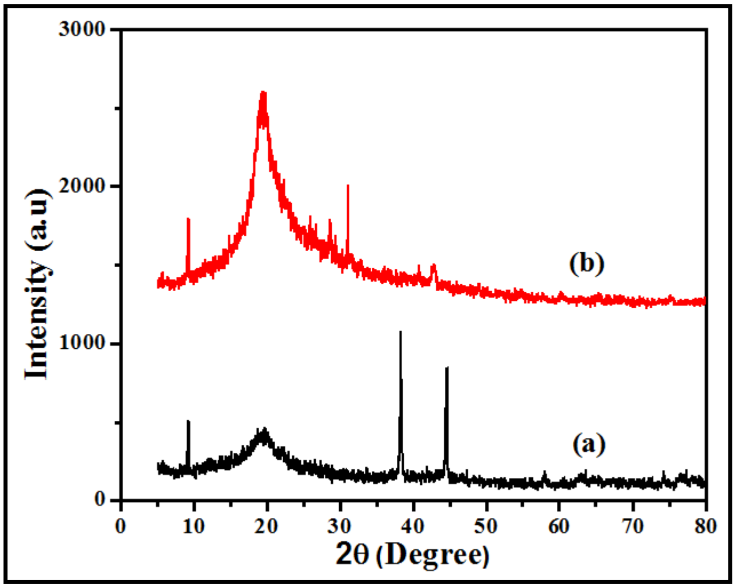

Figure S4: XRD of Ce-CHT/PVA composite nanofibers (a) before and (b) after adsorption of As (III)

To compare the quality of water subjected to experiments are tested before addition and after removal of As (III) were tested by UV visible spectrophotometer. The main purpose of this study was to check the solubility of Ce-CHT/PVA composite nanofibers, and remaining of As (III) if any in tested water. The UV-Vis spectra of tested water before and after As (III) removal were taken as given in (supplimentry information Fig .S5 (a) & (b)). The As (III) on adding in water shows peak 272 nm. No peak was observed in water having Ce-CHT/PVA composite nanofibers. To further substantiate the findings of AAS-HG, no peak was observed at 272nm after removal of As (III). UV-Vis spectra thus conclude that a Ce-CHT/PVA composite nanofiber removes As (III) efficiently.

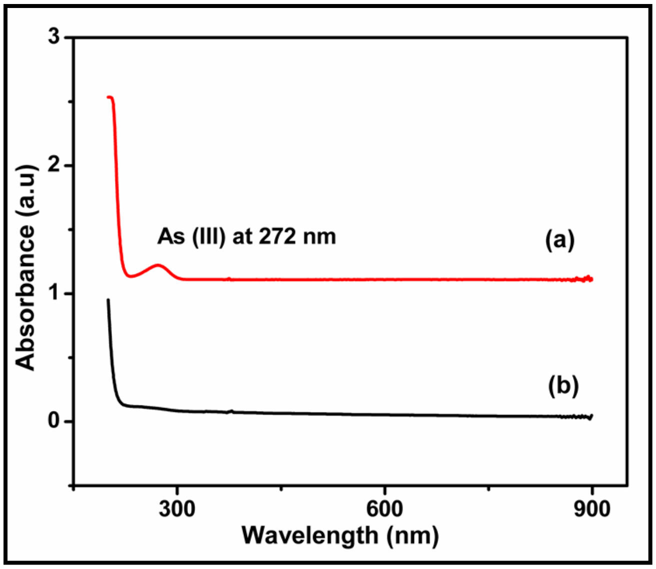

Figure S5. (a) UV-Vis spectra of Ce-CHT/PVA before and (b) after As (III) removal

Figure S6 (a) & (b) represents the effect of initial concentration on As (III) adsorption and Langmuir isotherm for bare CHT/PVA composite nanofibers respectively. As shown in the Fig 10 (a) adsorption capacity q_m (11.23mg/g) of bare CHT/PVA composite nanofibers is quite low. It is may be due to the fact that there is less positive charge on surface of bare nanofiber as compared to Ce-loaded CHT/PVA composite nanofibers.

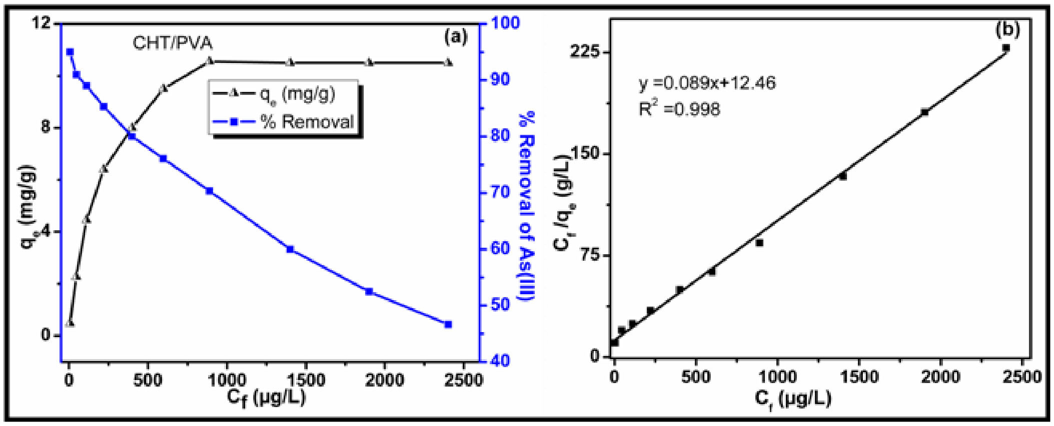

Figure S6: (a) Effect of initial concentration of As (III) on adsorption and (b) Langmuir adsorption isotherm for bare CHT/PVA composite nanofibers.