Electronic Supplementary Information (ESI)

Tailoring of Carbon Nanotubes for the adsorption of heavy metal ions: Molecular dynamics and experimental investigations

P. Sahu[1, 2], A.K. Singha Deb[1, 2], Sk. M. Ali[1,2*], K.T. Shenoy[1], S. Mohan[1]

[1]Chemical Engineering Division, Bhabha Atomic Research Center, Mumbai, Maharashtra, India 400085

[2] Homi Bhabha National Institute, Mumbai, Maharashtra, India 400094

***musharaf@barc.gov.in**

Fig S1. RDF profiles for (a) Cd^{++}-H_2O and (b) Cd^{++}-NO_3^- and corresponding coordination profiles for (c) Cd^{++}-H_2O and (d) Cd^{++}-NO_3^- in the aqueous phase in absence of CNT adsorbent.

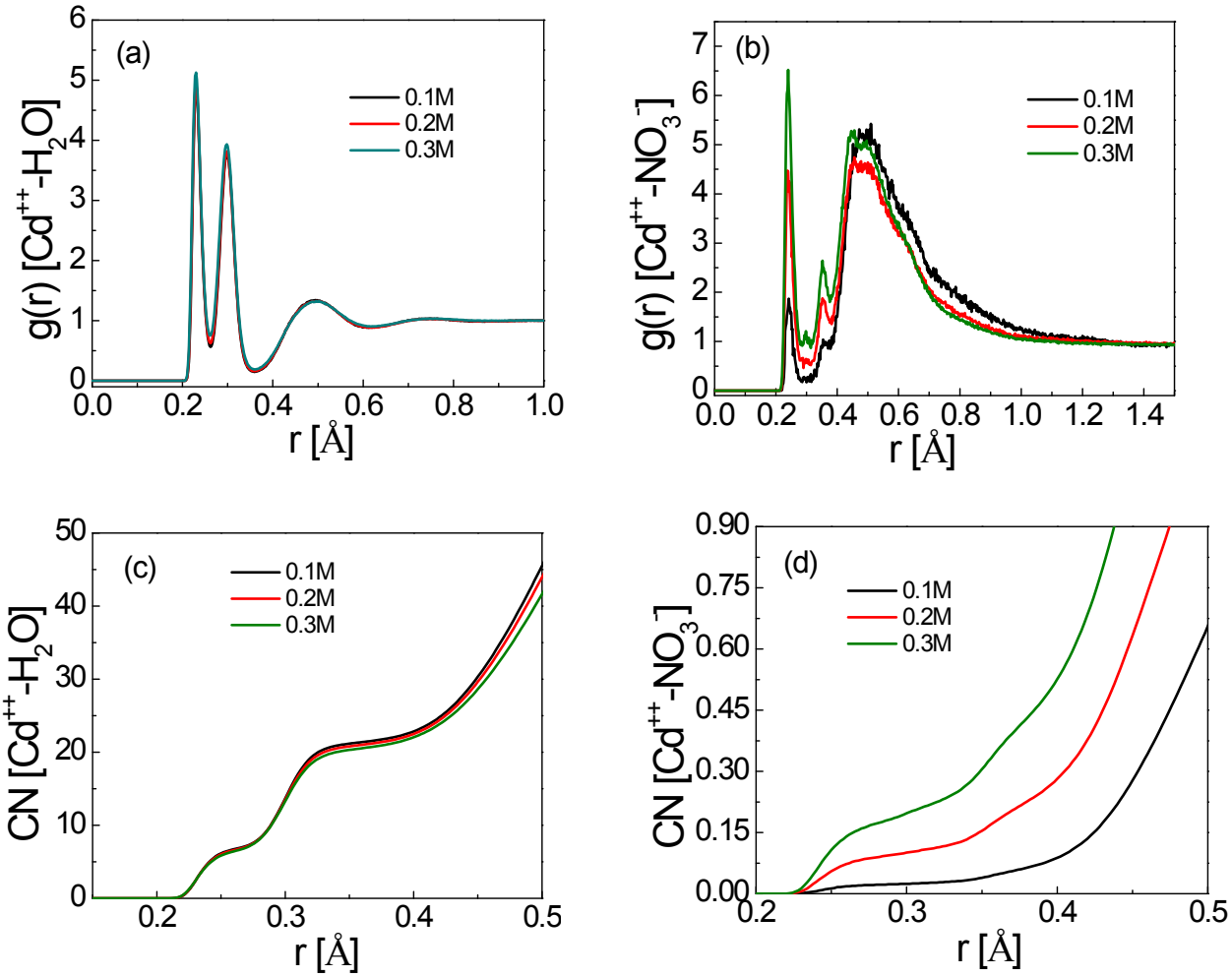
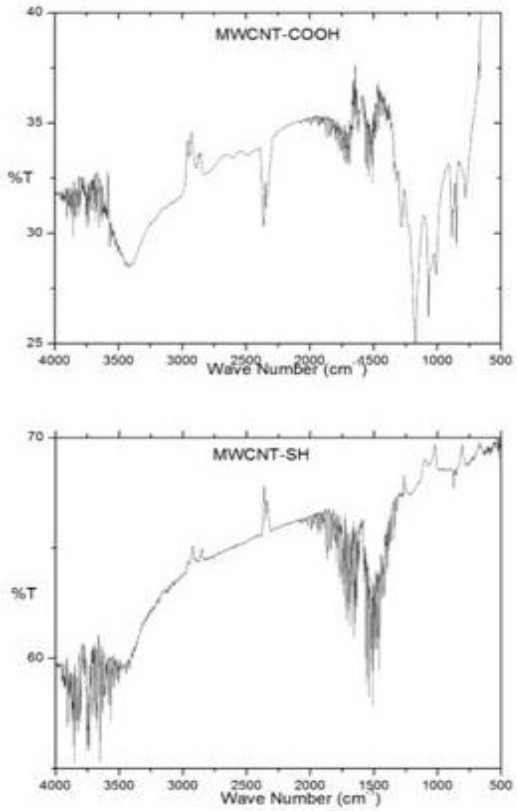


Fig. S2. FTIR spectra of MWCNT-COOH and MWCNT-SH



The presence of peaks at 3445 and 1650 cm^{-1} are related to the stretching vibrations of v(OH) and v(C=O) of the carboxyl groups (COOH), respectively. Symmetric and asymmetric methylene stretching bands at 2935 and 2891 cm-1, respectively, are observed to be present in the MWCNTs-COOH. It is assumed that defective sites on the sidewall of MWCNTs contain these groups.These characteristic peaks are presents for all the CNTs. The vibrational peak for C-S at 650-700 cm^{-1} along with amidic peak around 1642 cm^{-1} in the spectrum of MWCNT-SH suggest the attachment of –SH group through the amidic linkage with carboxyl of MWCNT-COOH and amine of cysteamine.