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Supporting information of "Templated Assembly of Metal Nanoparticles on DNA-SWCNT Hybrids Towards Optoelectronic Tunability"

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Experimental methods

DNA Strands used:

Table 1. DNA Sequences used throughout this study; all strands were obtained commercially from Integrated DNA Technologies (IDT).

	DNA Sequence (5'-3')
In-situ Wrapping	GTG TGT GTG TGT GTG TGT GTG TGT GTG TGT GTG TGT GTG T
Hybridisation Wrapping	TGC TAT GCA GCG GTC AAC TAC AGG CTC AGG
Non-Complementary Wrapping	TAT TAT TAT CGT TAG ATA CCG TAC CTC ACA TGC CAA C
Seeding Strand 1	CCT GAG CCT G
Seeding Strand 2	TAG TTG ACC G
Seeding Strand 3	CTG CAT AGC A

DNA Wrapping of SWCNTs:

To prepare DNA-wrapped SWCNTs, (6,5) Enriched SWCNTs (1 mg, Sigma Aldrich) were mixed with an aqueous dispersion of DNA (1 mL, 2 mg/mL ssDNA, IDT, 0.1M NaCl, Sigma Aldrich) via bath sonication (Branson 2800) in ice water for 90 minutes. The solution was then centrifuged (Biofuge pico D-37520, Heraeus Instruments) at 15,060 rpm for 60 minutes, with 70% of the supernatant extracted to be used. The DNA-CNT aqueous solution can then be stored at 4°C as a stock solution.

DNA Hybridisation Nanoparticles attachment on SWCNT:

The stock DNA-CNT solutions were first diluted 30-fold with 1x TAE. Dialysis against 1x TAE with Millipore dialysis membranes (100 kDa MWCO) was done to remove excess DNA. To seed the mini strand DNA, DNA (20 µL, 10 µM), MiliQ H_2O (30 µL), and M^{2+} (50 µL,10 mM, Pb^{2+} or Cd^{2+} or Ag^{+} prepared from $Pb(NO_3)_2$, $Cd(NO_3)_2$ or $AgNO_3$, Sigma Aldrich) were mixed and incubated overnight at 4 ºC. The seeded DNA solution (30 µL) was then added to the diluted DNA-CNT solution (150 µL) and incubated overnight. Finally, HS^- (5 µL, 10 mM, Na_2S, Sigma Aldrich) was added, followed by a further overnight incubation.

In-situ Nanoparticles Growth on SWCNTs:

The stock DNA-CNT solutions were diluted 10-fold with MiliQ H_2O. For each 10 µL aliquot of diluted DNA–CNT solution, Milli-Q H_2O (25 µL) and M^{2+} solution (10 µL, 5 mM; Pb^{2+}, Cd^{2+} or Ag^{+} prepared from $Pb(NO_3)_2$, $Cd(NO_3)_2$ or $AgNO_3$, Sigma-Aldrich) were added, and the mixture was incubated for 3 h. Subsequently, HS^- solution (10 µL, 5 mM Na_2S, Sigma-Aldrich) was added, followed by overnight incubation. The resulting metal sulfide–DNA–CNT solutions were then used for further characterisation.

Atomic force microscopy (AFM) Preparation:

Analysis of the SWCNT samples was done through AFM on a Bruker Dimension Icon in PeakForce Tapping mode with ScanAsyst Air tips. All AFM images were acquired at a scan rate of 0.977 Hz with a resolution of 512x512 pixels. The sample was prepared by depositing solution

onto freshly cleaved mica (5 µL), then incubating on a shaker for 10 minutes. The mica was then gently blow-dried using Argon (Ar) gas before washing with MiliQ H_2O (20 µL) and dried again.

AFM Statistical data acquisition:

AFM images were analysed to determine nanoparticle (NP) size distributions and NP surface densities along the SWCNTs. For each sample, multiple AFM images were acquired from independently prepared substrates to ensure reproducibility. Images were collected at different regions of the substrate to minimise sampling bias.

AFM data were processed using Nanoscope Analysis (Bruker, V 1.5), where height profiles were obtained utilising the cut tool. Individual NPs were identified based on height contrast relative to the SWCNT background. Height profiles were extracted along selected line sections to confirm the presence of nanoparticles and distinguish them from nanotube features. The coloured lines shown in the AFM images in the main text correspond to the positions where these height profiles were recorded.

For statistical analysis, NPs were manually counted and measured from multiple AFM images. In total, $N \approx 100$ were analysed per sample per method (PbS–SWCNT, CdS–SWCNT, and Ag_2S–SWCNT).

NP surface densities were calculated by counting the number of NPs associated with SWCNTs within a defined scan area and normalising by the total observable SWCNT length within that region. The reported values represent the mean values obtained from multiple images, with the associated standard deviations reflecting the variability between analysed regions.

AFM imaging was performed on multiple independently prepared samples, which consistently showed nanoparticle formation along the SWCNTs for all metal sulfide systems studied.

Optical Characterisation Techniques (UV-Vis, Raman, PL):

UV-Vis absorption spectra were recorded using a Shimadzu UV-3600 spectrometer. Raman spectroscopy was performed using a Renishaw inVia Raman microscope with a 532 nm laser excitation source (The Raman spectra presented represent the average measurements collected from at least three spatial locations per sample). Steady-state photoluminescence (SSPL) was carried out using an Edinburgh Instruments FLS1000 spectrometer with PMT-980 and NIR PMT-1400 detectors; excitation was provided by a 450 W ozone-free Xenon arc lamp.

Data acquisition and processing (UV-Vis, Raman, PL):

To assess reproducibility, each spectroscopic experiment was performed on at least three independently prepared samples. The spectra shown are representative of these measurements and were selected based on consistency in spectral features rather than optimal appearance. Averaging was applied only to repeated acquisitions of the same sample and not across different samples. No spectral manipulation beyond standard baseline correction and normalisation was performed for the UV-Vis spectra; a smoothing operation was applied to the PL spectra, with a Lorentz-Gaussian fitting applied to the Raman spectra.

Supplementary figures

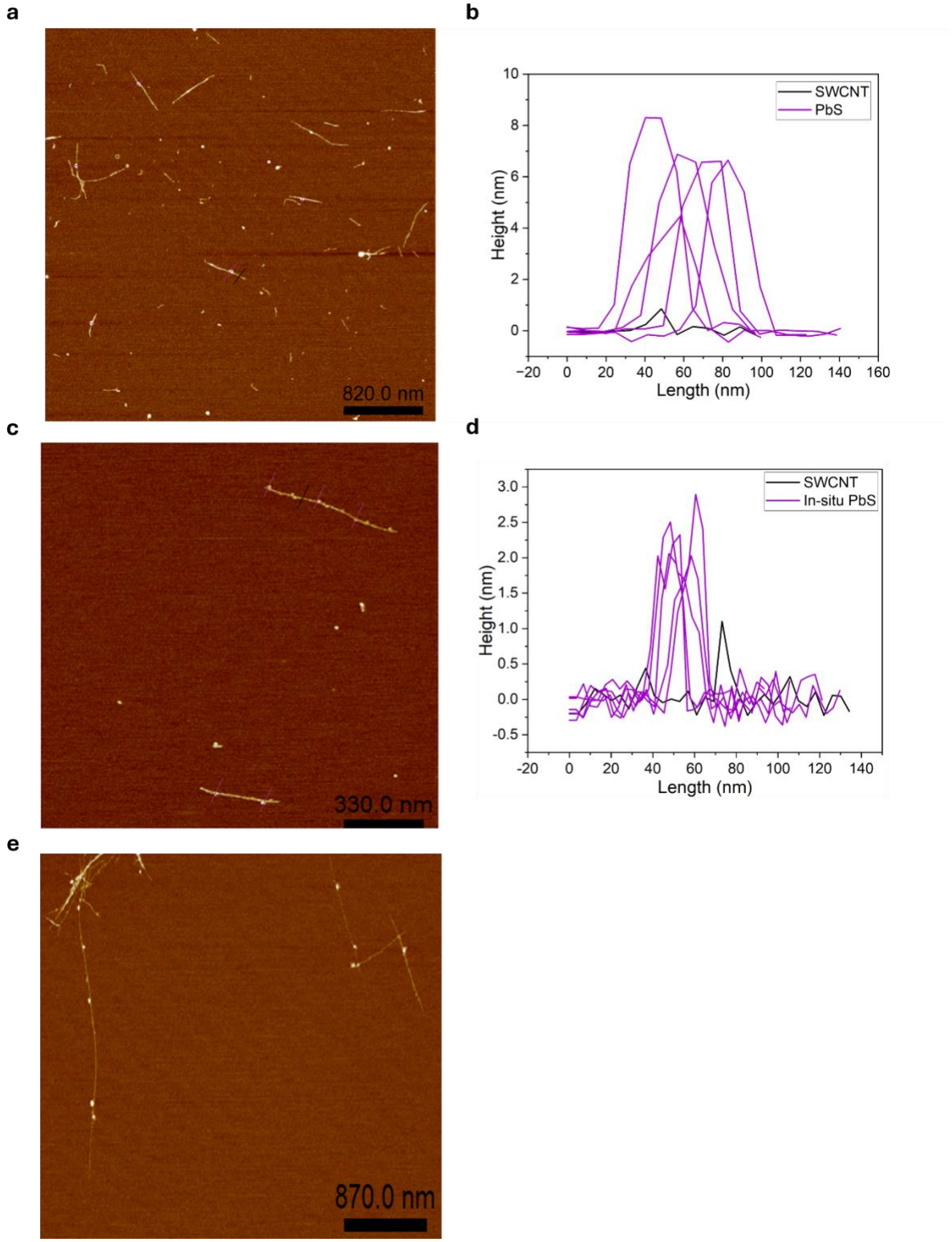

Figure S1: AFM images of DNA-wrapped (6,5) SWCNTs decorated with PbS NPs *via two methods. (a) DNA Hybridisation, (b) Height profile of the SWCNTs and the metal NPs. (c) In-situ method, (d) Height profile of the SWCNT and the metal NPs. (e) large-scale AFM image of in-situ seeded PbS NPs.*

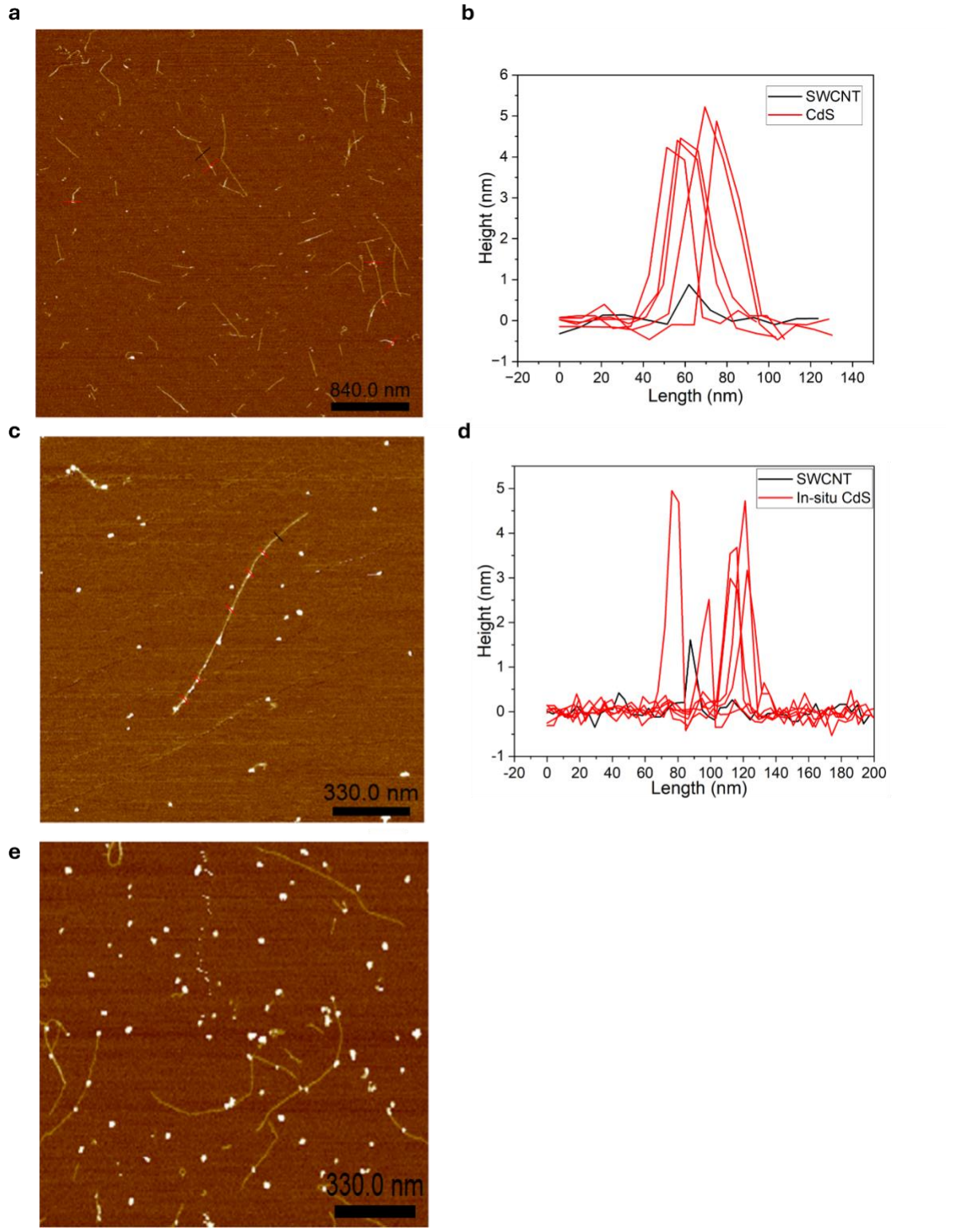

Figure S2: AFM images of DNA-wrapped (6,5) SWCNTs decorated with CdS NPs *via two methods. (a) DNA Hybridisation, (b) Height profile of the SWCNTs and the metal NPs. (c) In-situ method, (d) Height profile of the SWCNT and the metal NPs. (e) large-scale AFM image of in-situ seeded CdS NPs.*

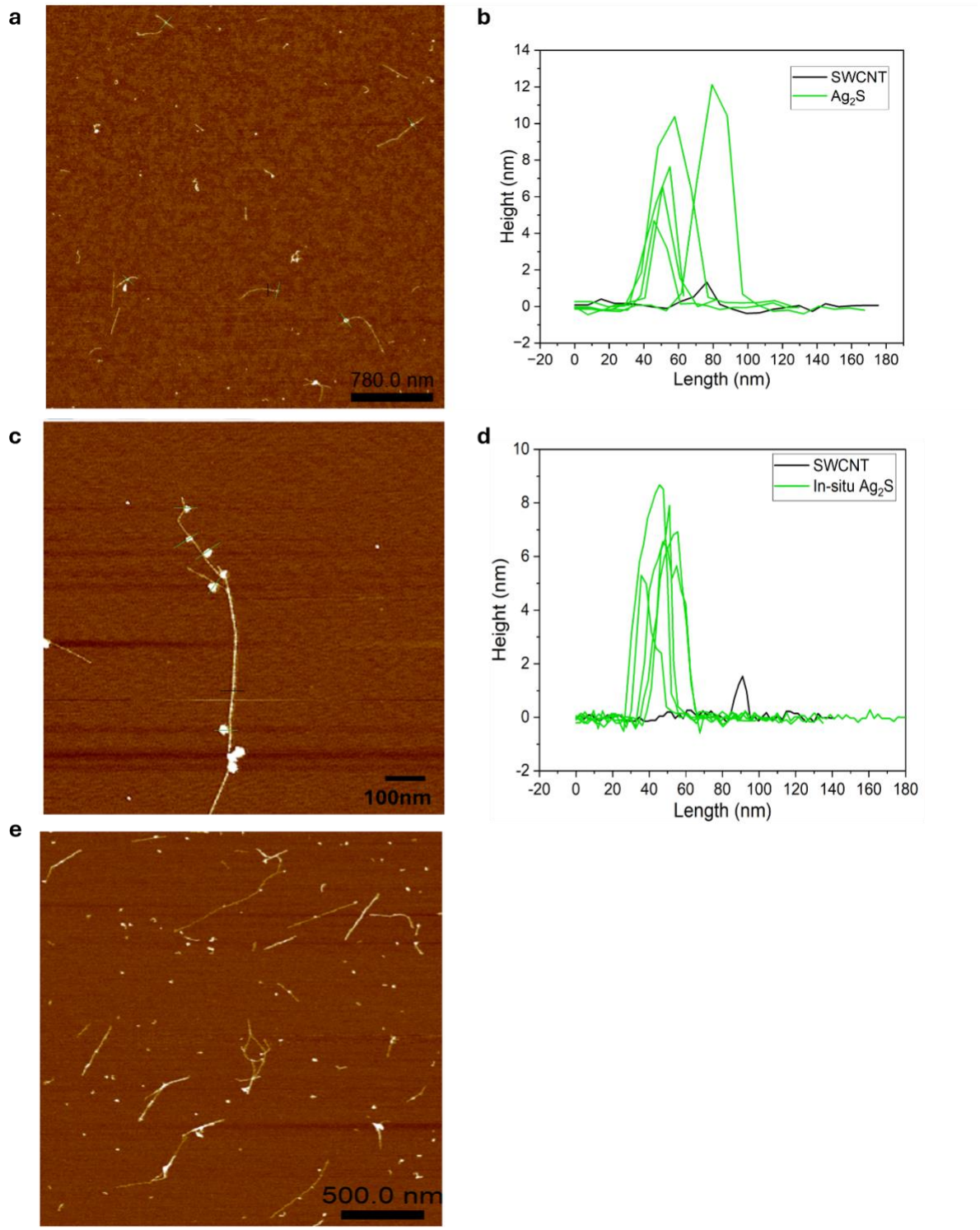

Figure S3: AFM images of DNA-wrapped (6,5) SWCNTs decorated with Ag_2S NPs *via two methods. (a) DNA Hybridisation, (b) Height profile of the SWCNTs and the metal NPs. (c) In-situ method, (d) Height profile of the SWCNT and the metal NPs. (e) large-scale AFM image of in-situ seeded* Ag_2S *NPs.*

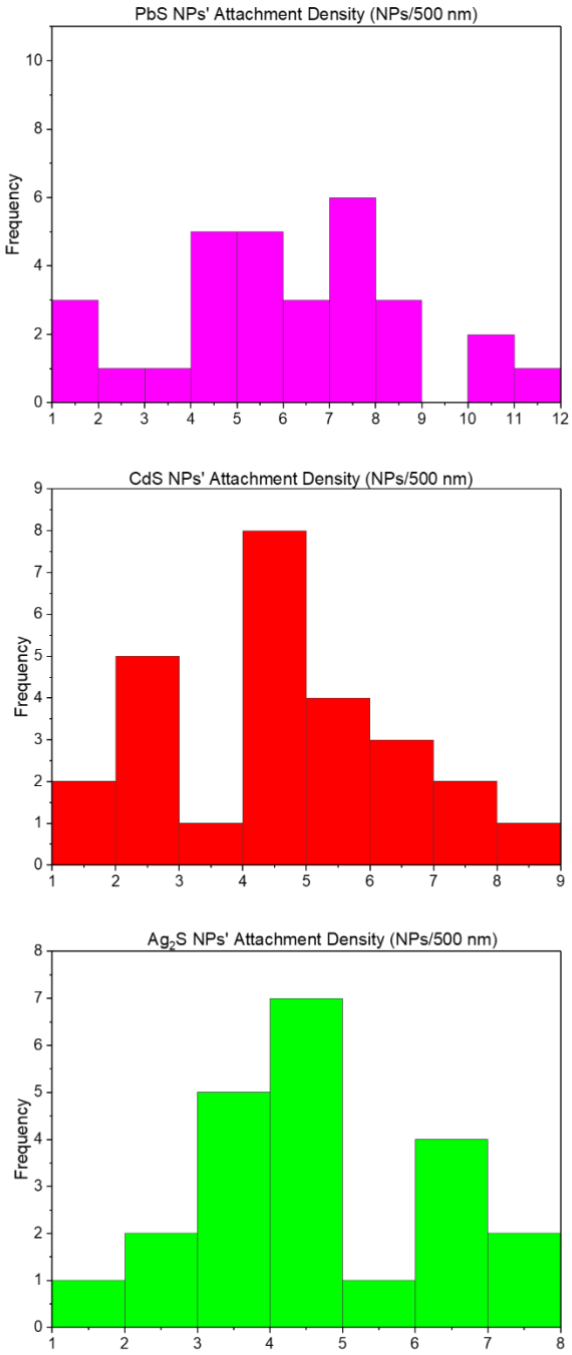

Figure S4: Frequency distribution of NPs density per 500nm of DNA-wrapped (6,5) SWCNTs length, resulting from the in-situ method. 30 counts were taken for PbS, 26 counts were taken for CdS, and 21 counts were taken for Ag_2S.

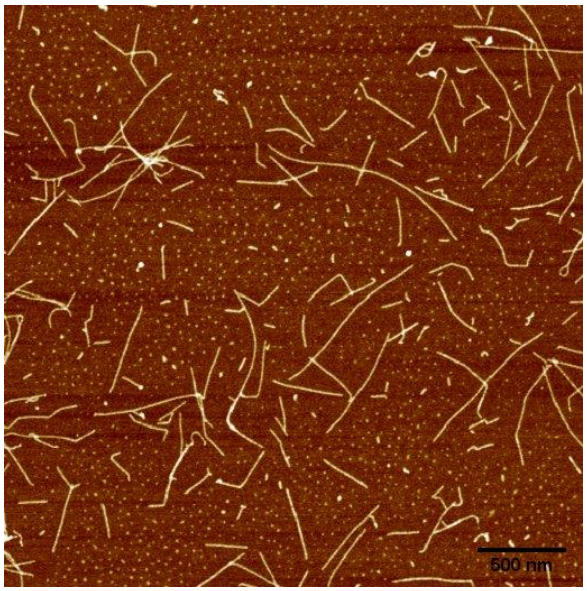

Figure S5: Use of non-complementary DNA-wrapped SWCNTs in the DNA hybridisation strategy. Without the duplex hybridisation, metal sulfide particles are not seen to attach onto the SWCNTs.

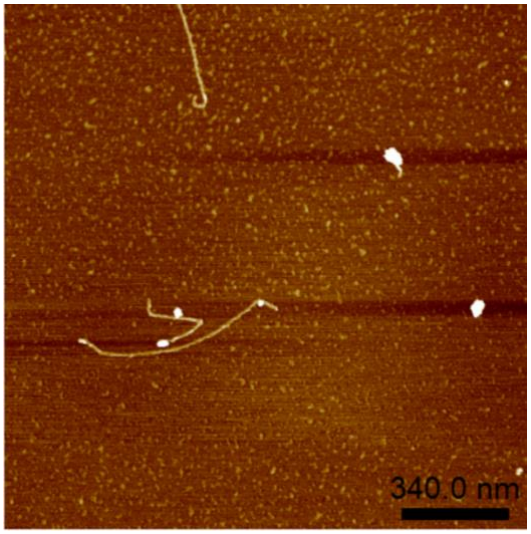

Figure S6: Pre-formed metal sulfide particle addition to DNA-wrapped SWCNTs. Large aggregates are seen, and no uniformly seeded SWCNTs are identified.

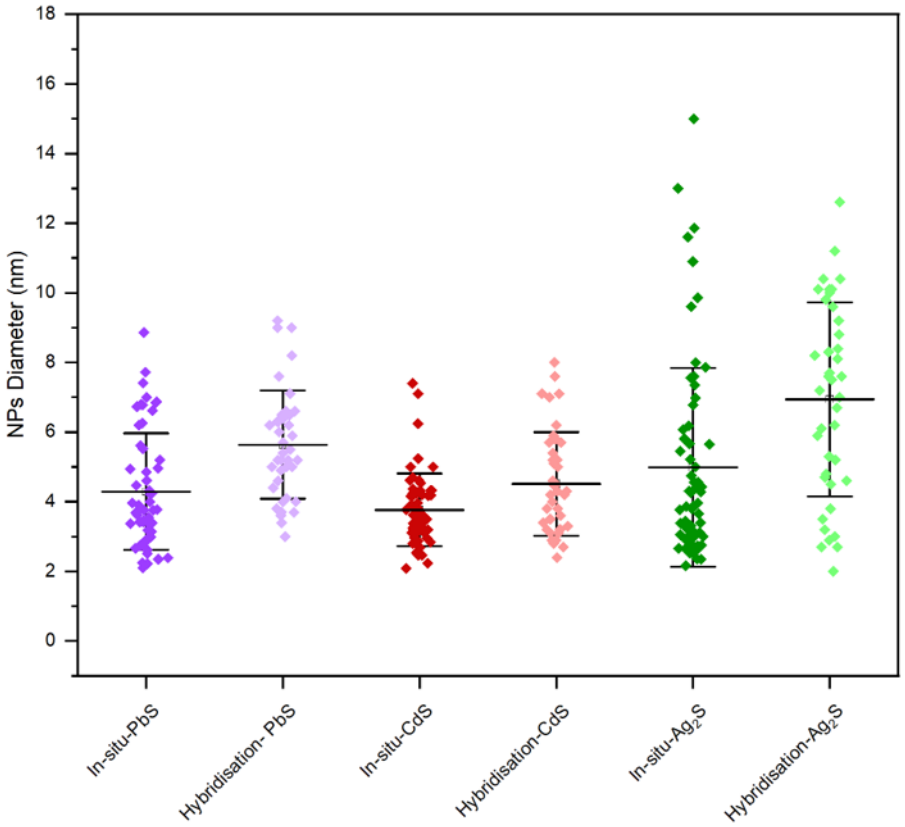

Figure S7: Nanoparticle size distribution between the two methods, larger NP sizes are seen for the DNA hybridisation method in comparison with the in-situ method.

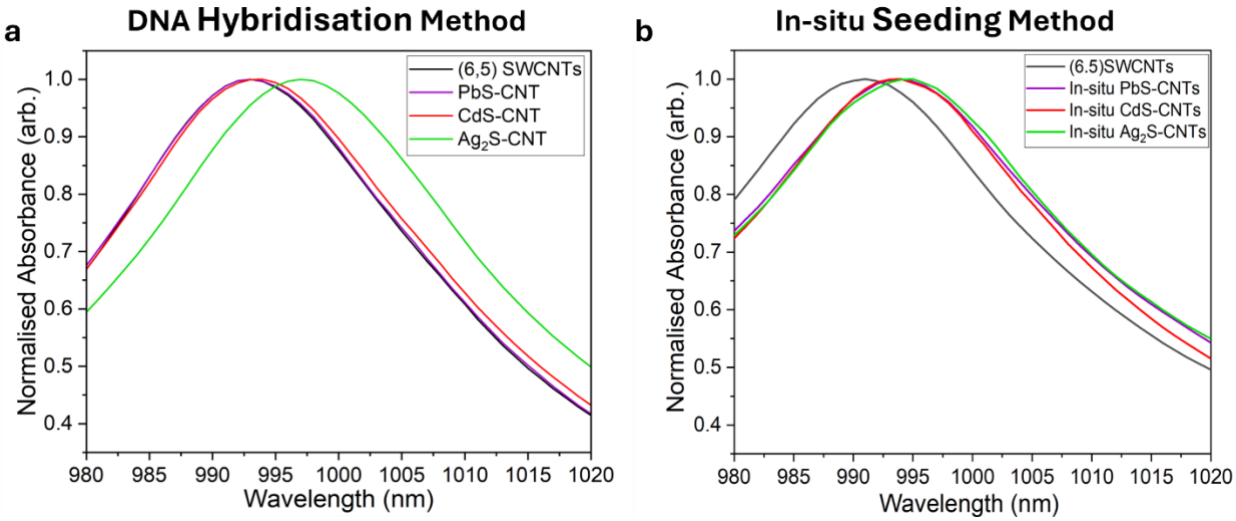

Figure S8: UV Spectroscopy of nanohybrids. (a) Excitonic peak (E_{11}) of the nanohybrids from the DNA Hybridisation method. (b) Excitonic peak (E_{11}) of the nanohybrids from the in-situ method.

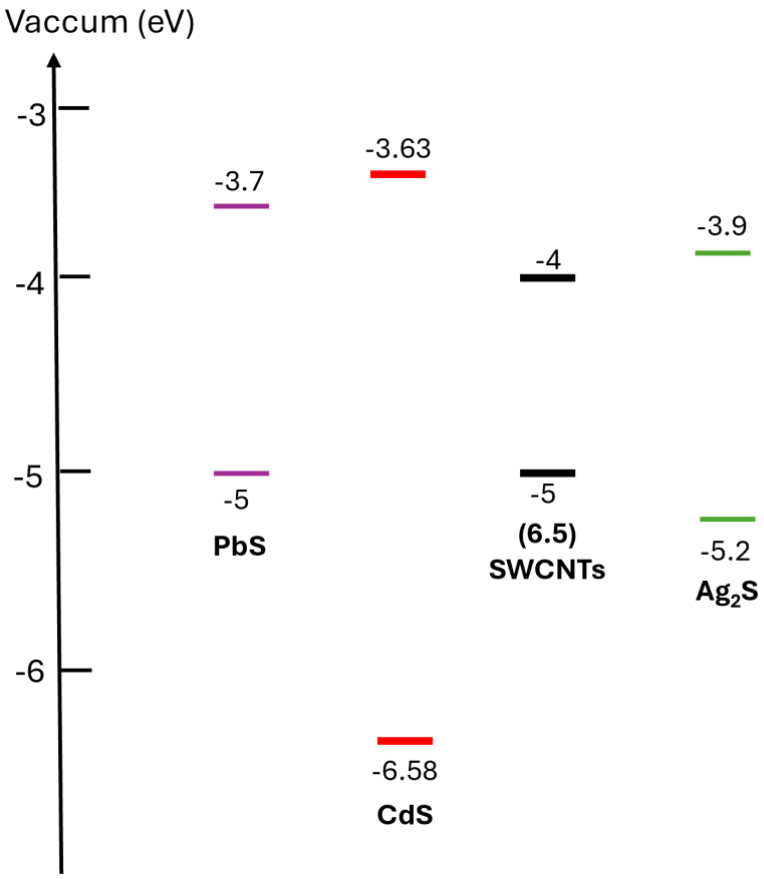

Figure S9: Band gap energy and relative band edge for the SWCNTs and the various nanoparticles used. The values of the work function are adapted from previous reports. [1–5]

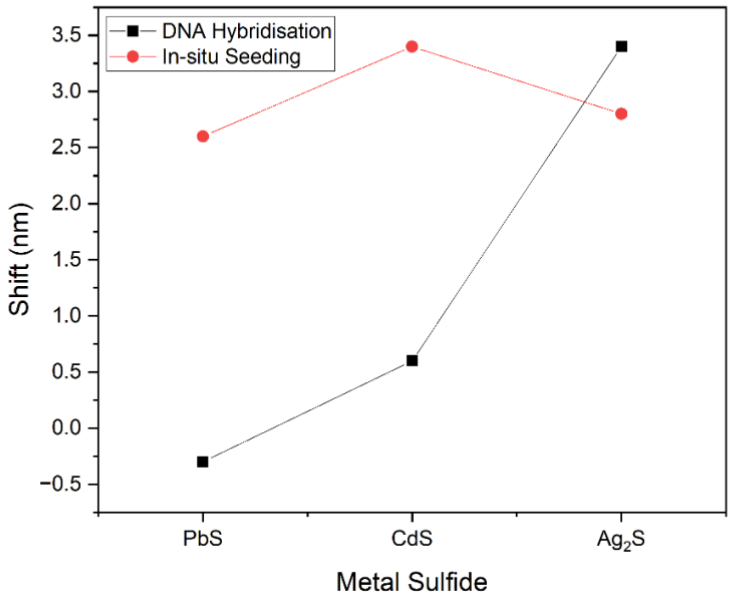

Figure S10: Photoluminescence spectra peak shift comparison between different metal sulfide nanoparticles, between the two different methodologies.

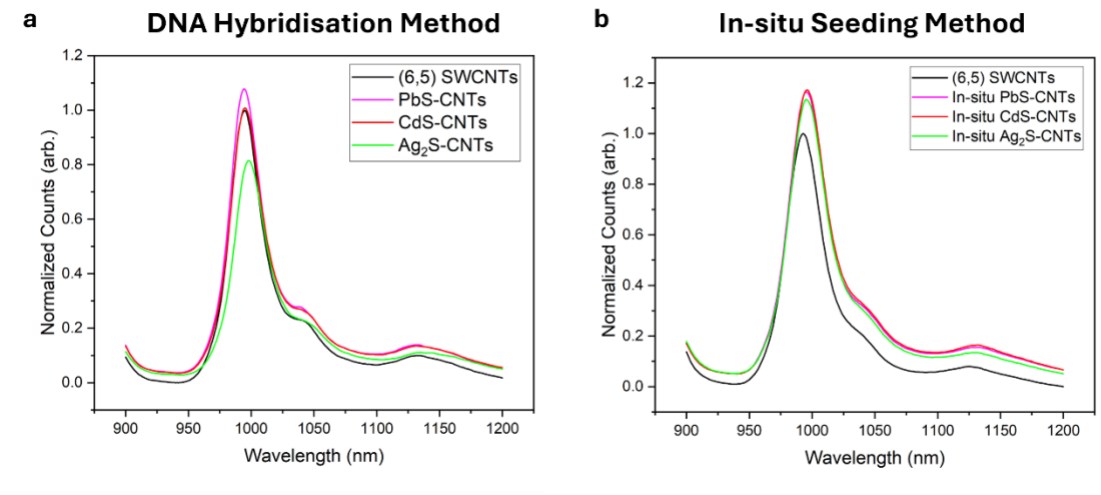

Figure S11: Steady-state photoluminescence characterization of SWCNT-based hybrids under 575 nm excitation obtained via the (a) DNA hybridisation and (b) in-situ methods

References

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