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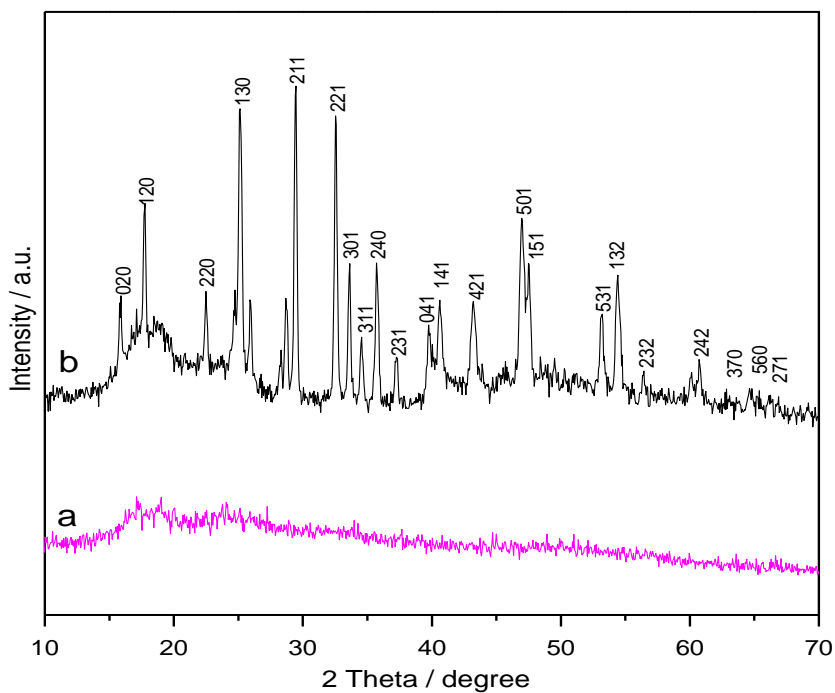
# Supplementary Information (SREP-12-03460)

## Controlled Assembly of $\text{Sb}_2\text{S}_3$ Nanoparticles on Silica/Polymer Nanotubes: Insights into the Nature of Hybrid Interfaces

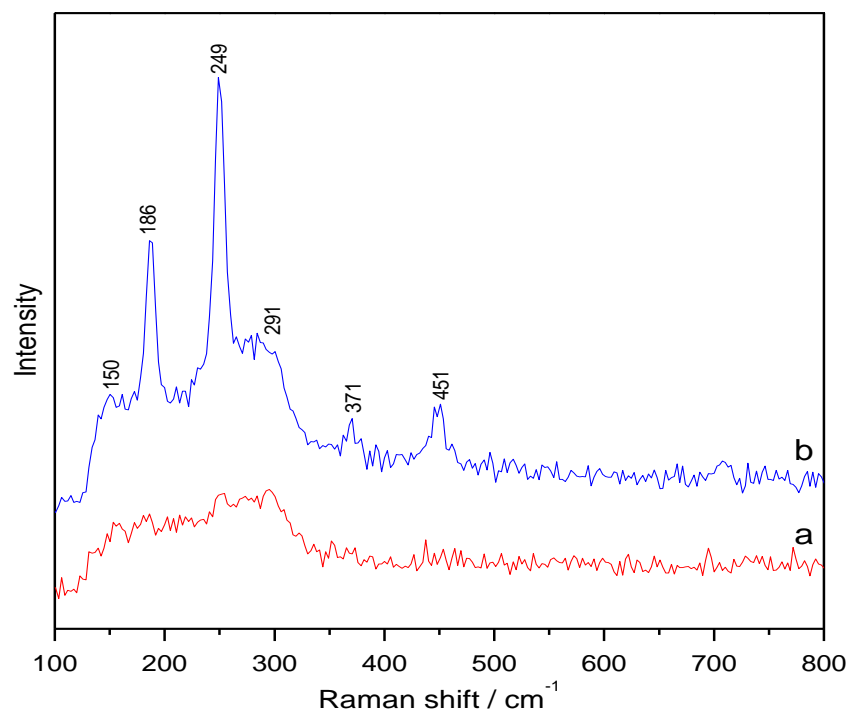
Huaming Yang, Mei Li, Liangjie Fu, Aidong Tang & Stephen Mann

**Table S1** Comparison of lattice parameters for various samples

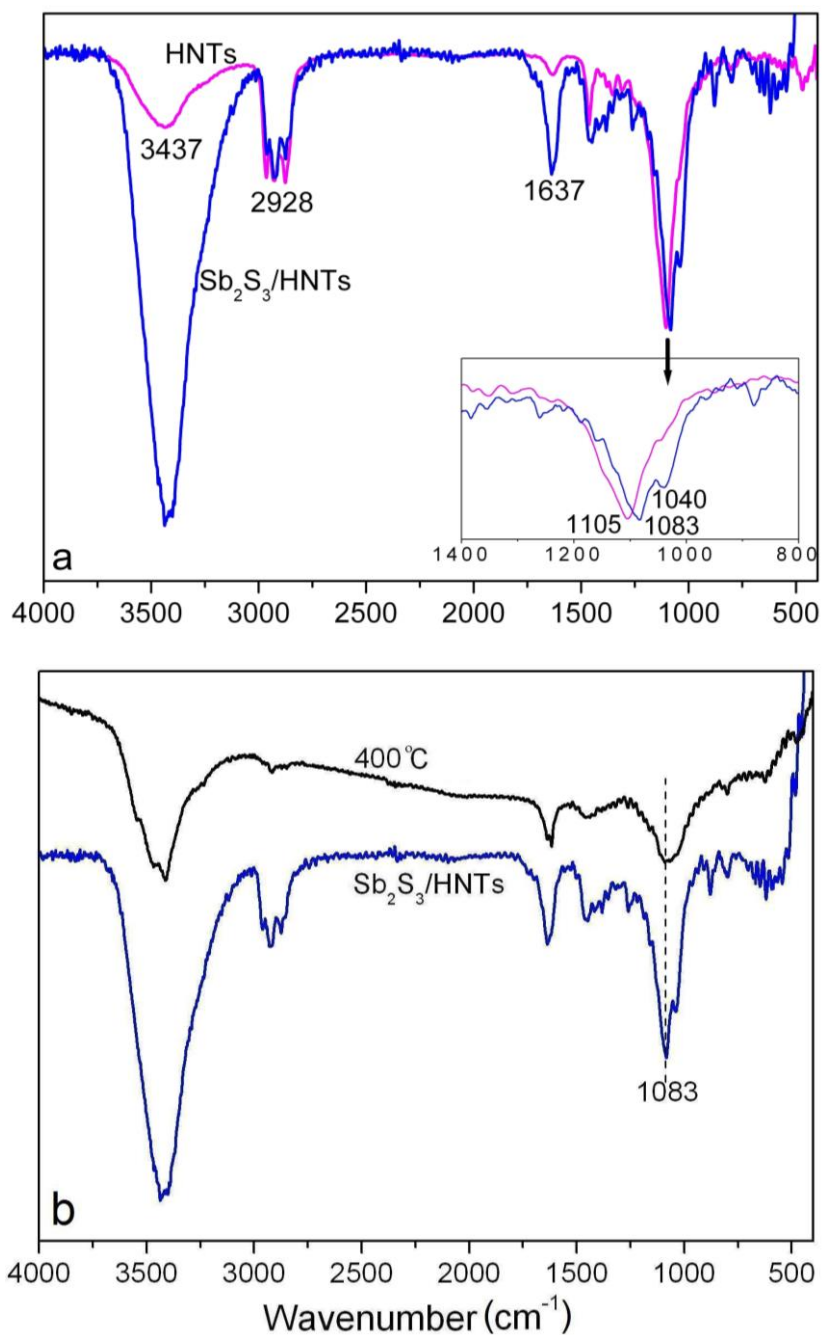
Sample	$a$ (Å)	$b$ (Å)	$c$ (Å)	Lattice volume (Å <sup>3</sup> )
calcined $\text{Sb}_2\text{S}_3$	11.226	11.321	3.838	487.81
calcined $\text{Sb}_2\text{S}_3/\text{HNTs}$	11.226	11.307	3.835	486.82
$\text{Sb}_2\text{S}_3$ (JCPDS 06-0474)	11.229	11.310	3.839	487.55



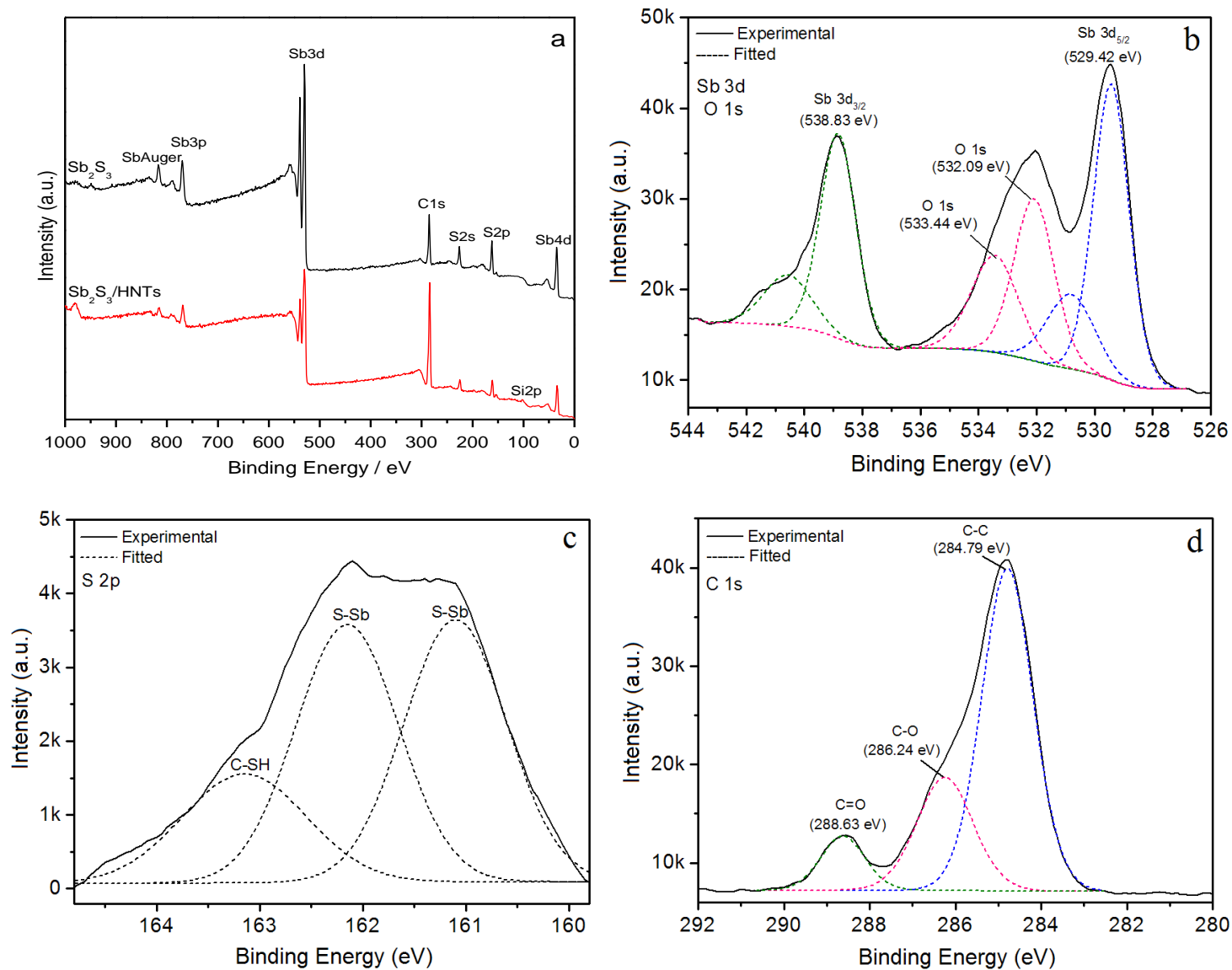
**Figure S1** XRD patterns of (a) as-synthesized  $\text{Sb}_2\text{S}_3$  and (b) calcined  $\text{Sb}_2\text{S}_3$  at 400 °C under  $\text{N}_2$ .



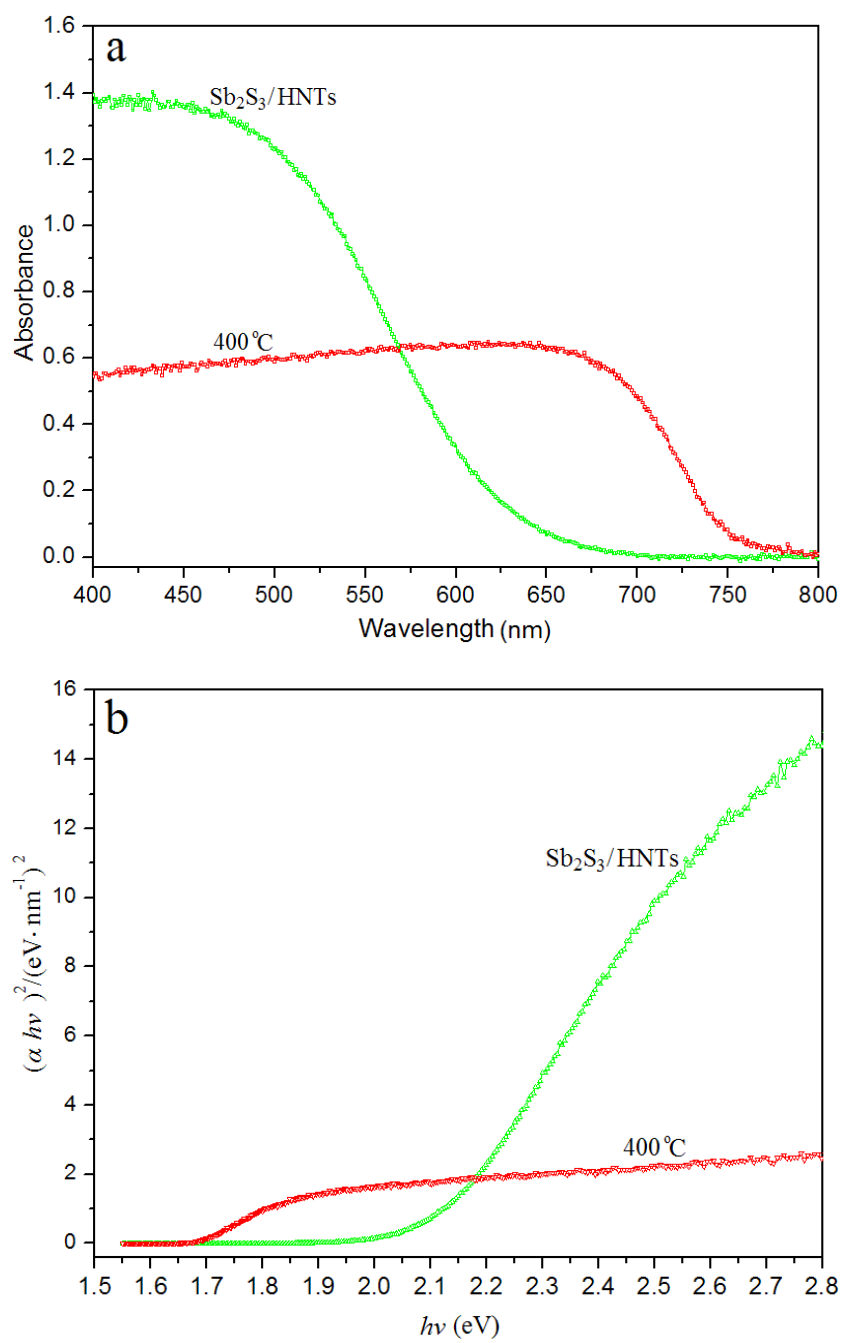
**Figure S2** Raman spectra of (a) as-synthesized Sb<sub>2</sub>S<sub>3</sub>/HNTs and (b) heated Sb<sub>2</sub>S<sub>3</sub>/HNTs at 400 °C under N<sub>2</sub>.



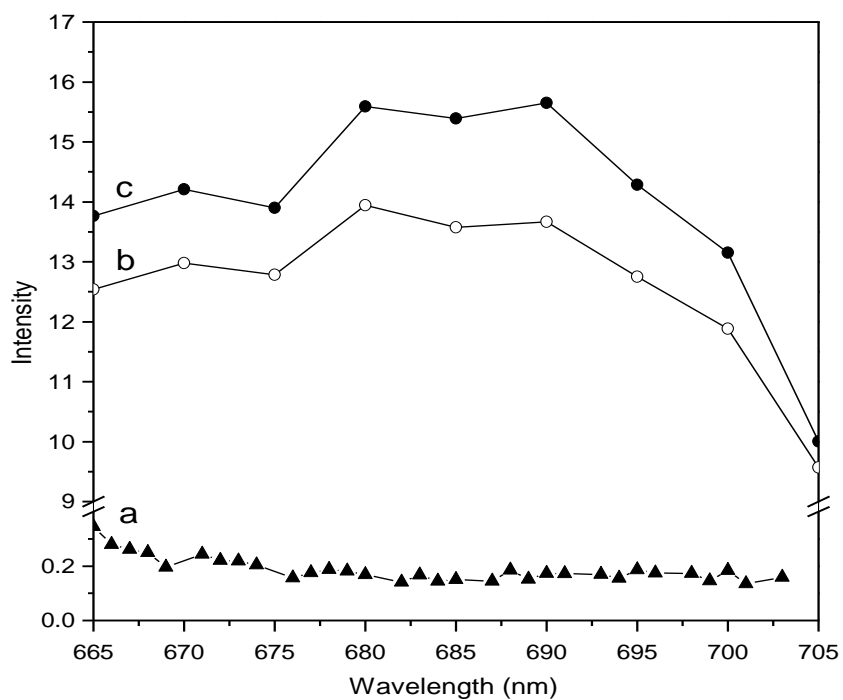
**Figure S3** (a) FTIR spectra of HNTs and as-synthesized  $\text{Sb}_2\text{S}_3/\text{HNTs}$ . The large increase in the intensity of the O-H and -NH<sub>2</sub> stretching vibrations at 3437  $\text{cm}^{-1}$ , and C=O stretching vibration at 1637  $\text{cm}^{-1}$ , as well as the appearance of a C-N stretching vibration at 1040  $\text{cm}^{-1}$ , is associated with the acetamide byproduct of the reaction of TAA with antimony chloride. (b) FTIR spectra of as-synthesized  $\text{Sb}_2\text{S}_3/\text{HNTs}$  and calcined  $\text{Sb}_2\text{S}_3/\text{HNTs}$  at 400 °C under N<sub>2</sub>.



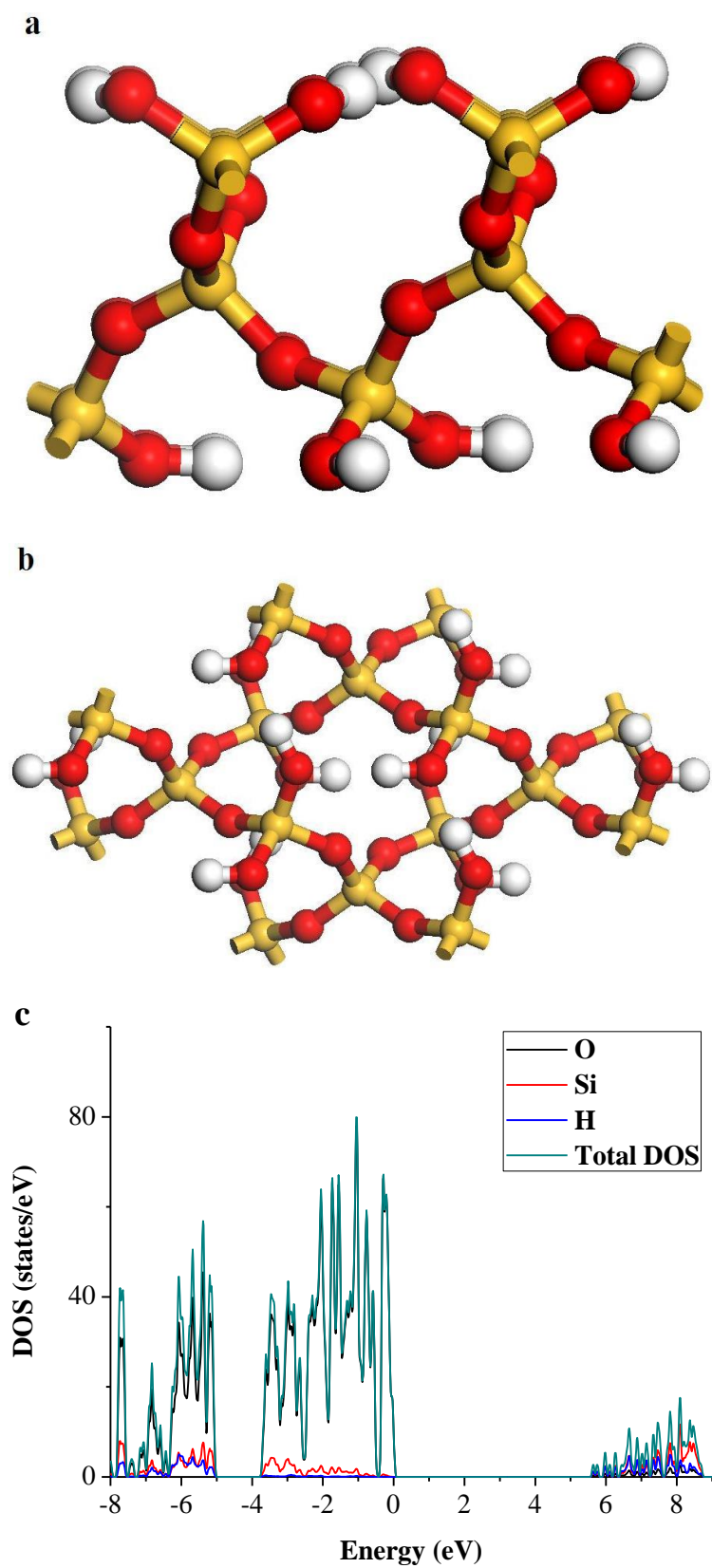
**Figure S4** (a) XPS survey spectra of the as-synthesized  $\text{Sb}_2\text{S}_3$  and  $\text{Sb}_2\text{S}_3/\text{HNTs}$ . Trace amounts of carbon in the control sample originate from residual impurities during the synthesis procedure. High-resolution XPS profiles and fitted lines for (b) Sb 3d and O 1s, (c) S 2p and (d) C 1s regions for as-synthesized  $\text{Sb}_2\text{S}_3/\text{HNTs}$ .



**Figure S5** (a) Solid-state UV-vis spectra and (b) plots of  $(\alpha hv)^2$  versus  $hv$  of as-synthesized  $\text{Sb}_2\text{S}_3/\text{HNTs}$  and the calcined  $\text{Sb}_2\text{S}_3/\text{HNTs}$  at  $400^\circ\text{C}$  under  $\text{N}_2$ .

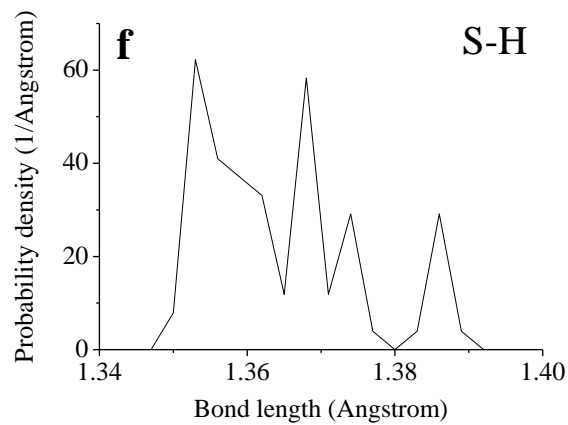
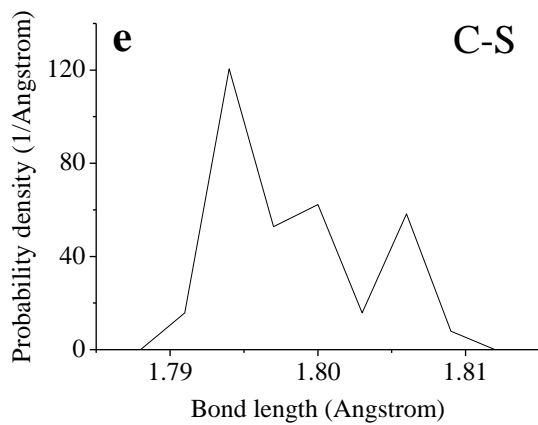
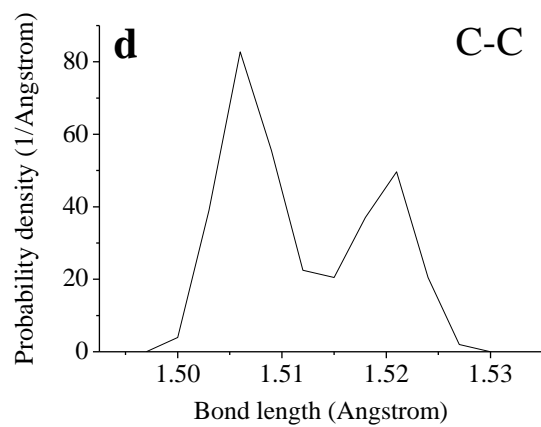
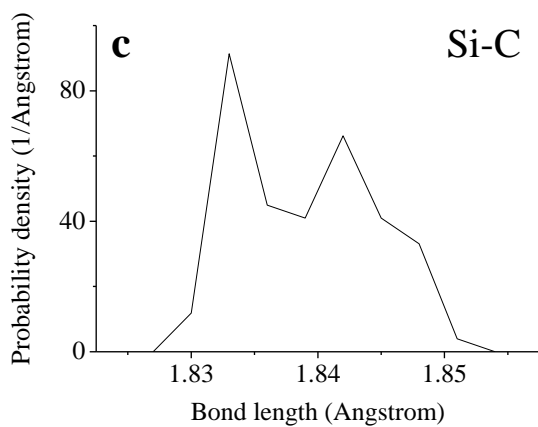
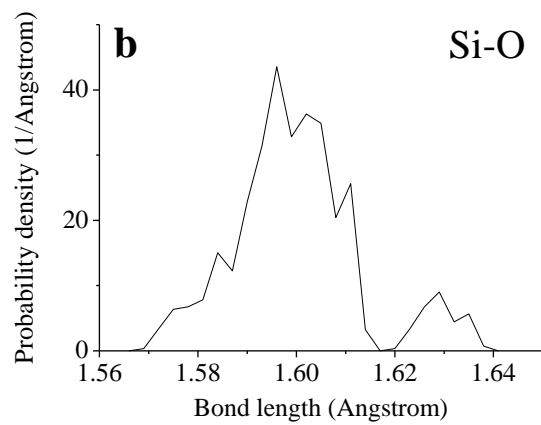
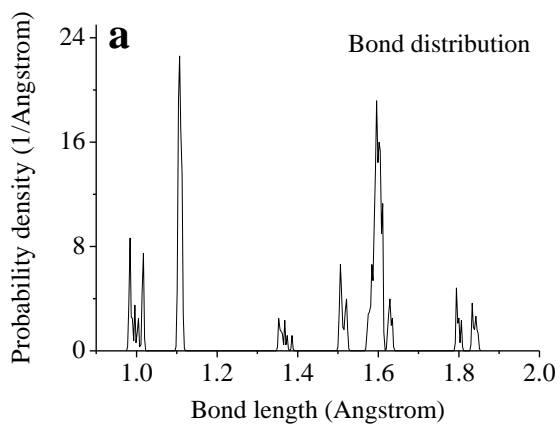


**Figure S6** Fluorescence spectra of (a) original HNTs, (b) as-synthesized  $\text{Sb}_2\text{S}_3$  and (c)  $\text{Sb}_2\text{S}_3/\text{HNTs}$ .

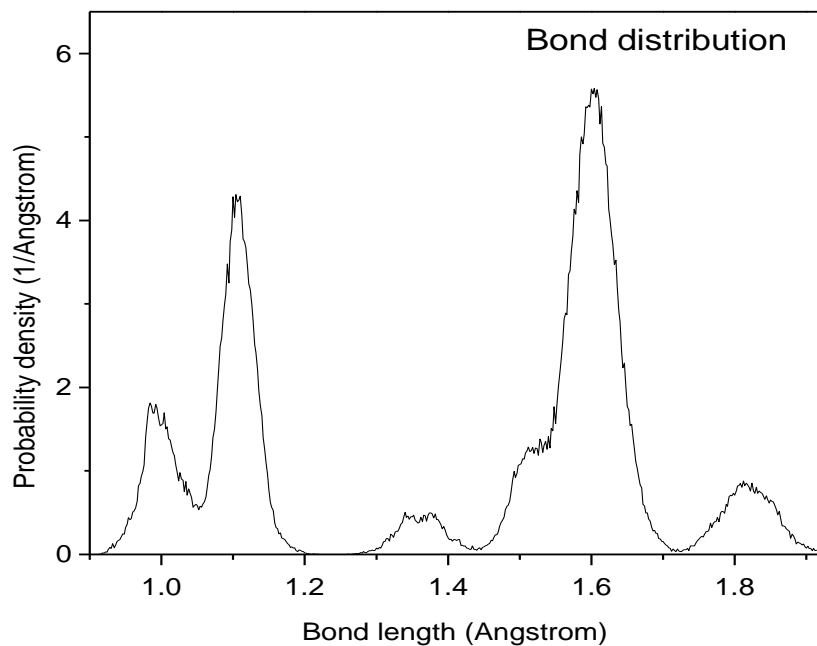


**Figure S7** Structural model of amorphous silica surface. (a) Side view, (b) top view, and (c) corresponding total density of states (DOS) and atom-projected density of states (PDOS).

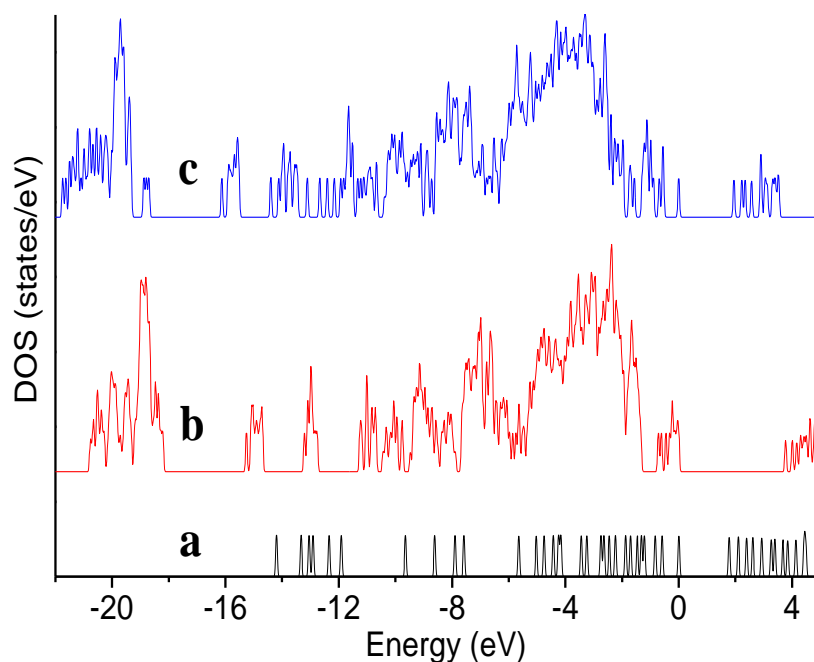




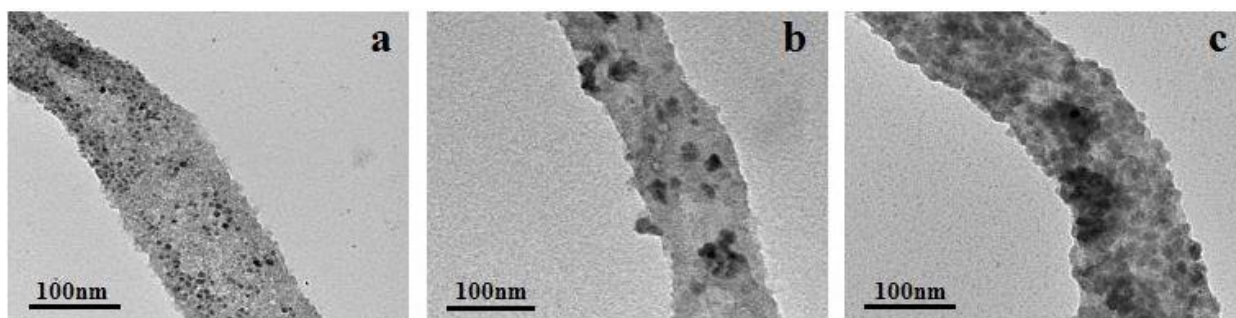
**Figure S8** Bond length distributions of the HNTs surface.



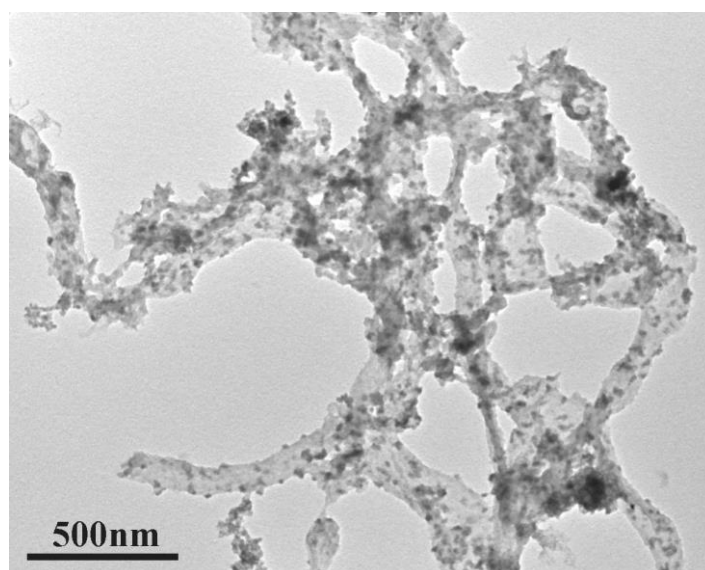
**Figure S9** Bond length distribution on a mercaptopropyl-functionalized amorphous silica surface after 5 ps dynamic equilibrium.



**Figure S10** Total density of states (DOS). The calculated band gaps were: (a) pure  $\text{Sb}_2\text{S}_3$  (1.75 eV), (b) mercaptopropyl-functionalized silica surface (HNTs, 3.75 eV), and (c)  $\text{Sb}_2\text{S}_3$ /HNT nanocomposites (2.0 eV). The latter two values agreed well with the experimental results (solid-state UV-vis spectroscopy, Figure S5). The underestimate of the band gap is mainly due to the well-known LDA problem, but it does not influence the theoretical analysis.



**Figure S11** TEM images of the individual HNT coated with  $\text{Sb}_2\text{S}_3$  nanoparticles for the as-synthesized  $\text{Sb}_2\text{S}_3/\text{HNTs}$  prepared by simultaneously adding TAA and HNTs to a  $\text{Sb}(\text{III})$  solution at  $\text{Sb}:\text{Si}$  molar ratio of (a) 1:1 and (b) 1:10. (c) Sample prepared by adding TAA followed by a HNTs suspension.



**Figure S12** Low magnification TEM image of as-synthesized  $\text{Sb}_2\text{S}_3/\text{HNTs}$  at  $\text{Sb}:\text{Si}=1:10$ .