

Supplementary Information

Selective extraction of metallic arc-discharged single-walled carbon nanotubes by a water soluble polymethylsilane derivative

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1. Synthesis of polymethylsilane

Polymethylsilane was prepared by a sodium-mediated Wurtz reductive coupling of dichloromethylsilane in refluxing toluene.¹ 23 g (1.0 mol) new cutting sodium metal was drastically stirred to sodium sand in 500 ml toluene under N₂ atmosphere at 100°C, and then 52.5 ml (0.5 mol) dichloromethylsilane was added drop by drop. After refluxing for 9 h at 115 °C, the reactant mixture was filtered with normal filter paper to get rid of sodium residues. The filtrate was evaporated with a rotary evaporator to remove unreacted dichloromethylsilane and toluene solvent, and then polymethylsilane was obtained as a light yellow viscous liquid.

2. The relative purity of the semiconducting SWNTs (S₂₂)

An estimate of the relative abundance of metallic and semiconducting SWNTs can be derived by integrating the peak areas in the M₁₁ and S₂₂ regions, and the purity ratio of semiconducting SWNTs in the supernatants could be calculated as ²

$$R_{\text{Sem}} = 1/(1 + I_{\text{M11}}/I_{\text{S22}})$$

where I_{M11} and I_{S22} are the integrated peak areas in the M₁₁ and S₂₂ regions, respectively. As show in Fig. S1 the ratios of the areas under the curves after and before baseline subtraction, AA(S)/AA(T) are 0.191 and 0.138 for the DOC-SWNTs and the complex polymethyl(1-undecylic acidyl)silane and SWNTs, respectively. Therefore, the relative carbonaceous purity of the SWNTs dispersed with polymethyl(1-undecylic acidyl)silane to that of SWNTs dispersed with DOC is ~ 0.72 (0.138/0.191). The content of the semiconducting-SWNTs is 47.3% for the complex polymethyl(1-undecylic acidyl)silane and SWNTs, but 76.1% for DOC-SWNTs by calculating , which indicates the percent content of semiconducting-SWNTs were reduced. Therefore polymethyl(1-undecylic acidyl)silane has good separation of metallic-SWNTs but not semiconducting-SWNTs from as-produced SWNTs.

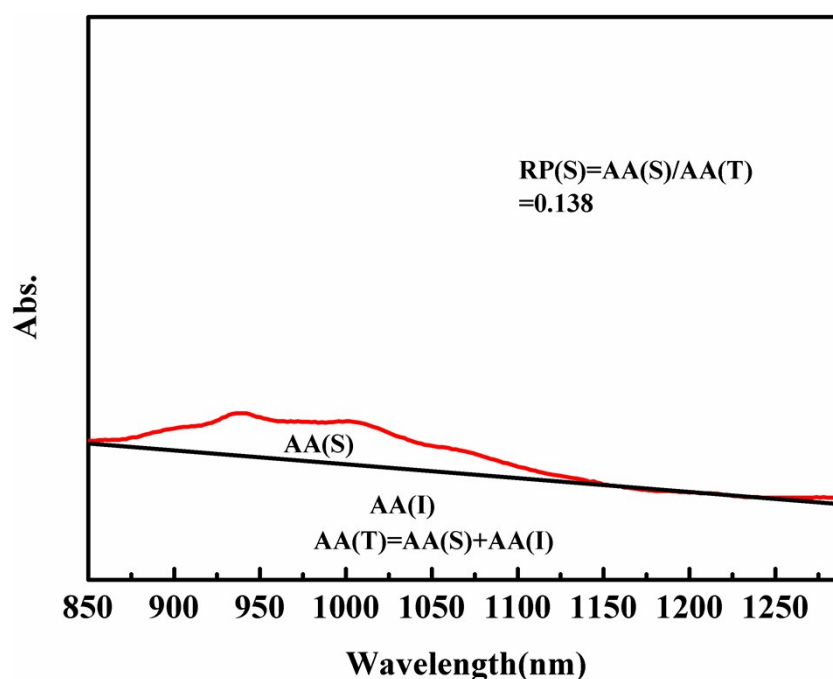
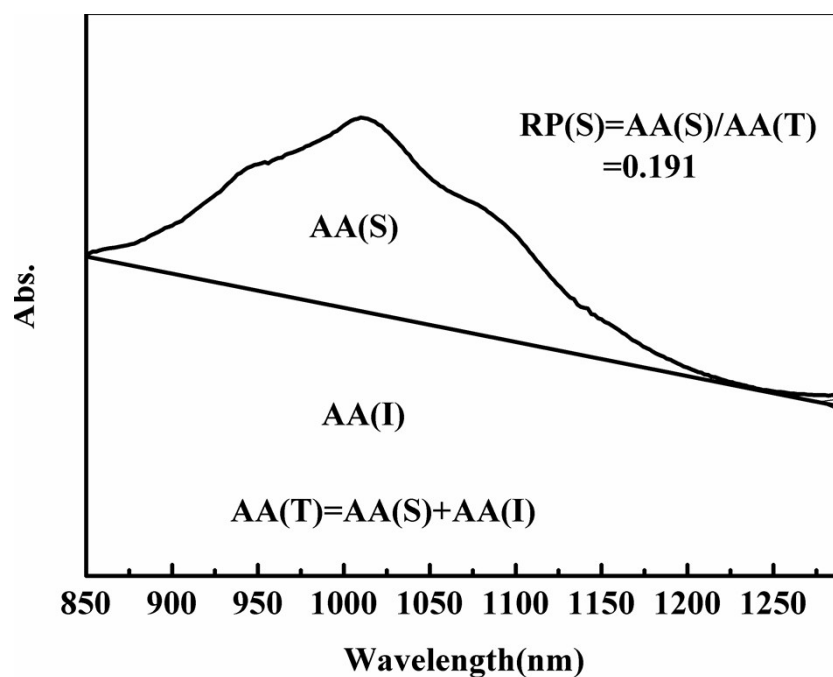


Fig. S1 The relative purity of DOC-SWNTs (upper) and the complex of polymethyl(1-undecylyl)silane and SWNTs (lower) based on the vis-NIR absorption spectra .

3. The self-assembly of the complex of polymethyl(1-undecylyl)silane and SWNTs

Shown in Fig. S2 and Fig. S3 are the SEM and AFM images of the complex of polymethyl(1-undecylyl)silane and SWNTs, which were placed 30 days, dropped and dried on Si wafer and then stoved at 100 °C for 12 h. It is obvious that the SWNTs in the supernatants are free from

metal catalyst particles and carbonaceous particles, since most of them are deposited into the precipitate. On the other hand, big bundles of SWNTs are observed to be coated with blurred materials and branch cross-linked to some extent. It is no doubt that these blurred materials are self-assembled polymethyl(1-undecylic acidyl)silane, indicating that they are wrapped onto the surface of carbon nanotubes as time goes on. The branch cross-linked appearance is assume to be formed from these well dispersed larger bundles of SWNTs about 2 μm length. During the preparation of SEM and AFM samples, they aggregate to larger bundles under the driving of the self-assembly of polymethyl(1-undecylic acidyl)silane, being observed as rigid structures.³

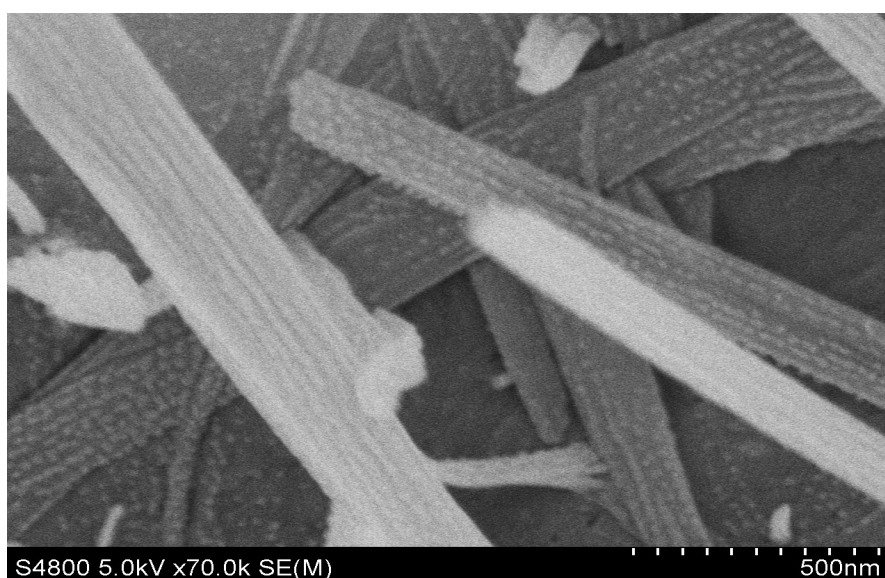
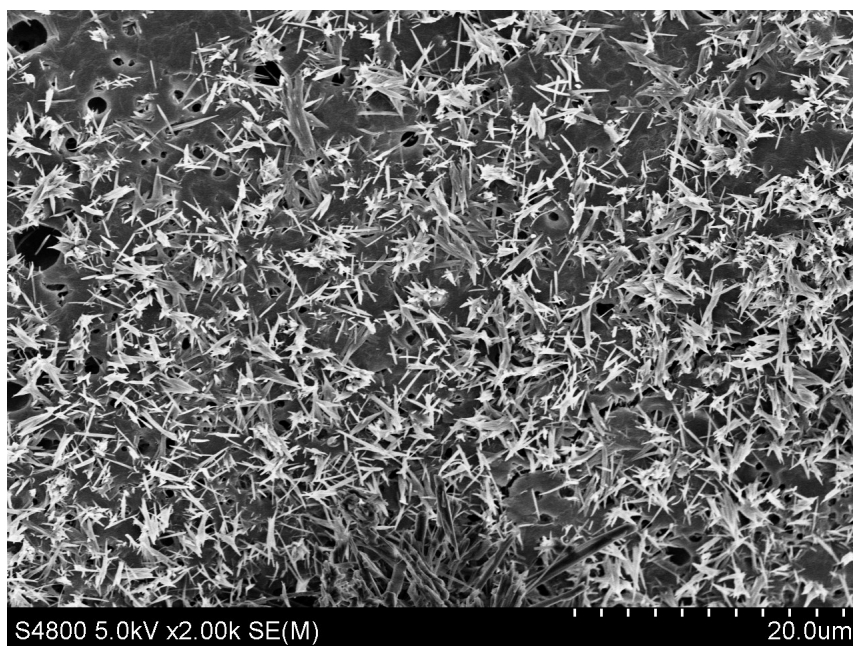


Fig. S2 The SEM images of the complex of polymethyl(1-undecylic acidyl)silane and SWNTs taken after setting for 30 days.

4. TEM image of the complex of polymethyl(1-undecylic acidyl)silane and

metallic-SWNTs.

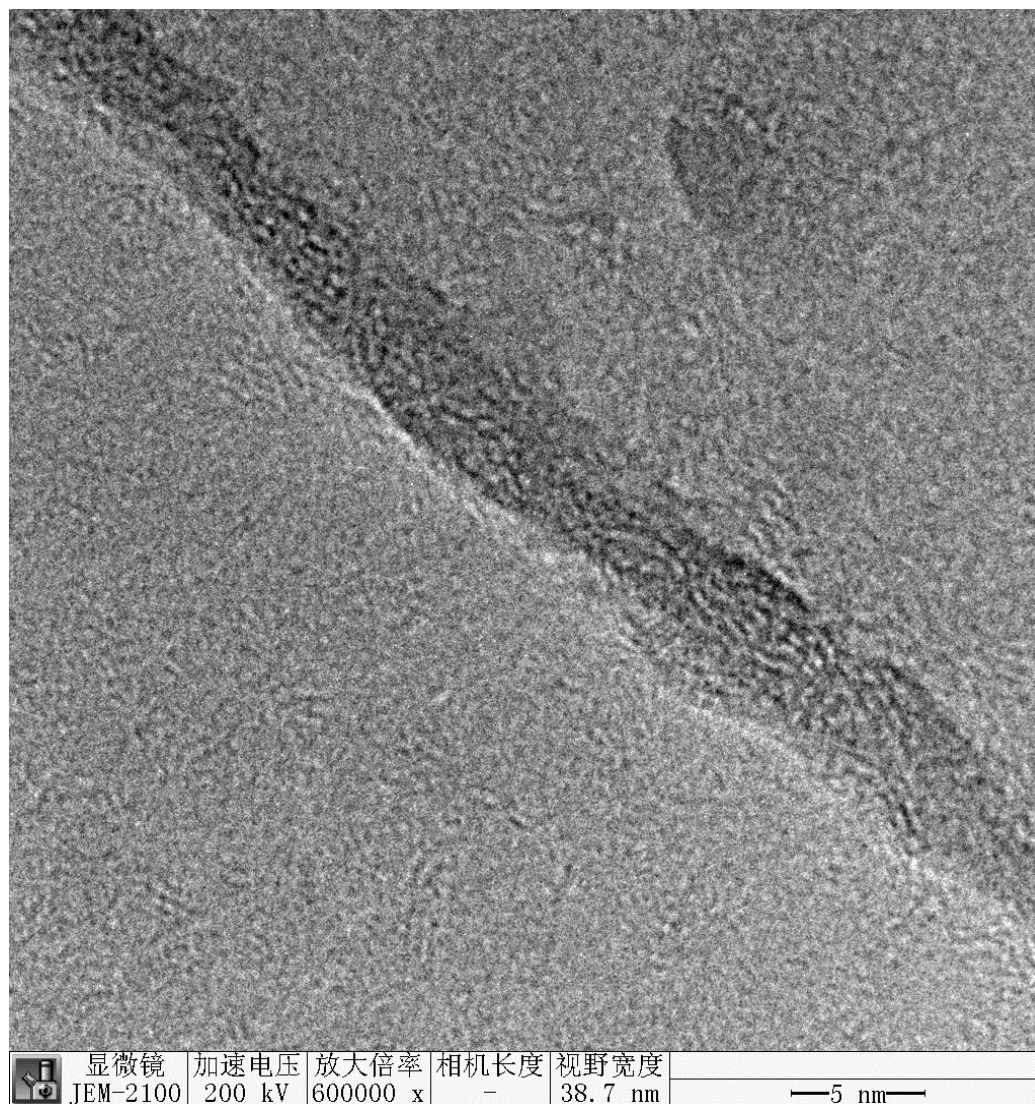


Fig. S3 The TEM image of the complex of polymethyl(1-undecylyl)silane and SWNTs.

References

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