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Supporting Information

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Evidence of Diamond Nanowires Formed inside Carbon Nanotubes from Diamantane Dicarboxylic Acid**

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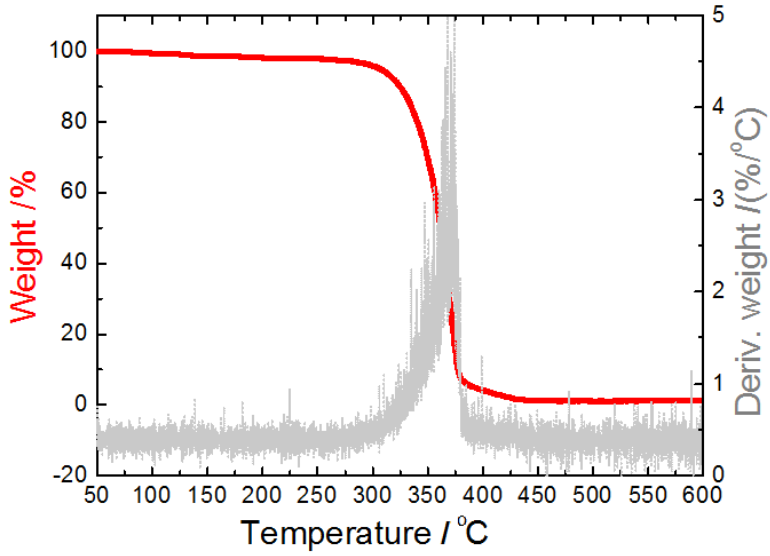

Figure S1. Thermogravimetric analysis **(**TGA) data of 4,9-diamantane dicarboxylic acid in air.

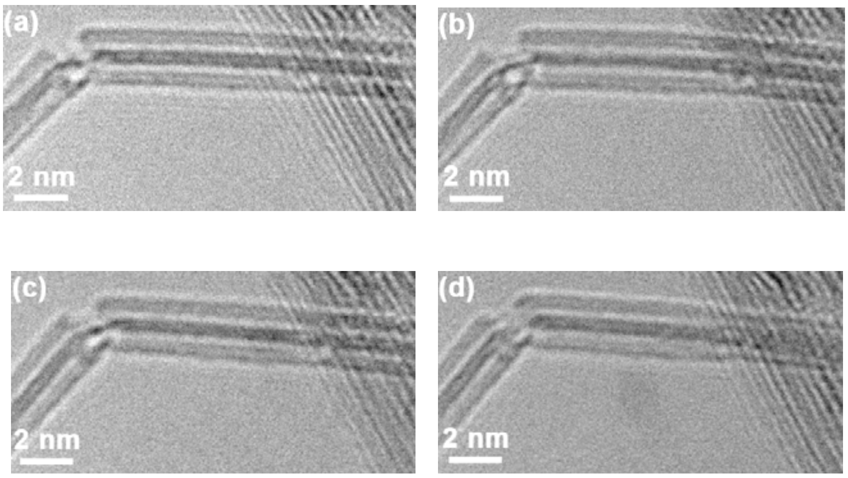

Figure S2. HR-TEM observation of carbon-based nanowires inside a DWCNT exposed to electron beam irradiation for around (a) 5 min, (b) 10 min, (c) 20 min, and (d) 30 min. Under these experimental conditions, enclosed nanowires may encounter tensile forces exceeding 23 nN that, according to our calculations, may break the nanowire.

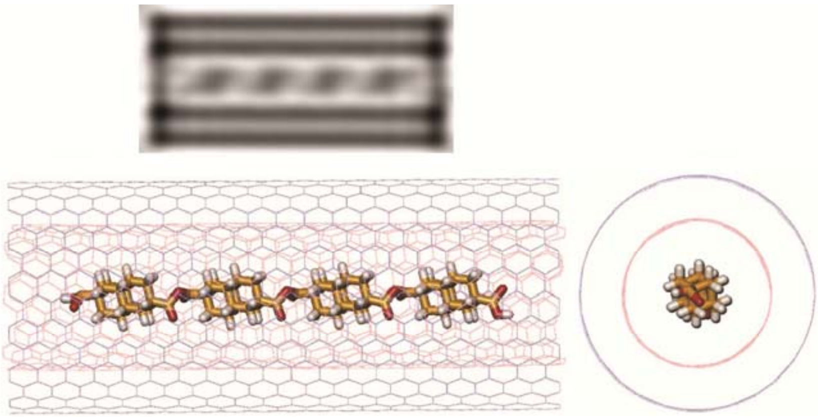

Figure S3. Simulated TEM image and underlying model structure of a diamantane anhydride polymer in a DWCNT.

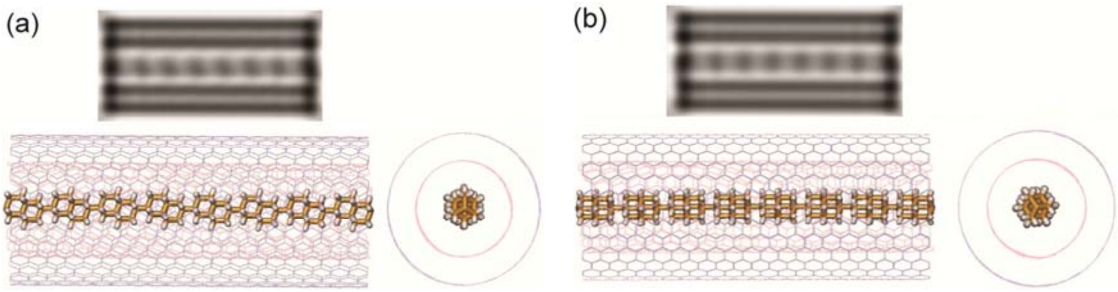

Figure S4. Simulated TEM images and underlying model structure of a diamantane polymer in DWCNTs.

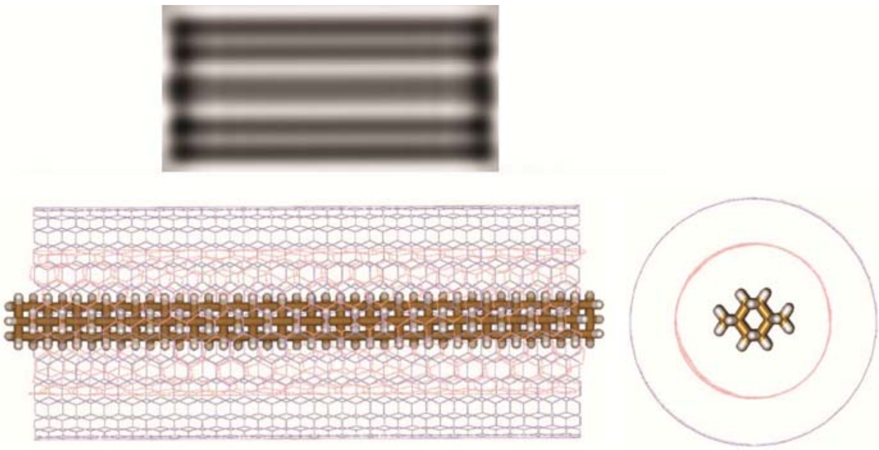

Figure S5. Simulated TEM image and underlying model structure of a diamond nanowire with the (100) crystal face inside a DWCNT.

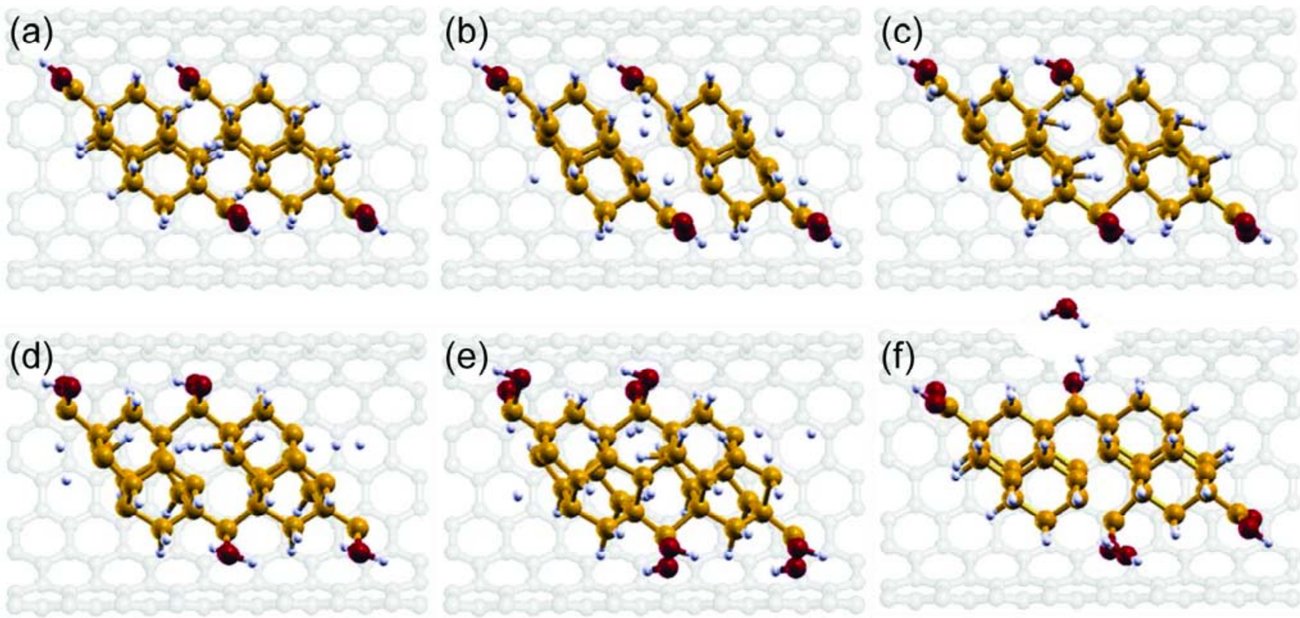

Figure S6. Snapshots of molecular dynamics simulations representing key steps leading to the fusion of 4,9-diamantane dicarboxylic acid molecules inside an (8,8) carbon nanotube. (a) Initial structure of adjacent molecules, constrained to a 5 Å center-to-center distance. Detachment of H atoms from carbon atoms at the interface in (b) leads to the formation of a new C-C bond connecting neighboring molecules in (c). Next, hydrogen attaches to one of the terminal oxygen atoms, converting it to an OH radical (d). Further hydrogenation of the two OH radicals connected to a carbon atom (e) causes the conversion to and detachment of water molecules (f). Hydrogenation of the terminal C atom completes the conversion of adjacent 4,9-diamantane dicarboxylic acid molecules to a diamond nanowire segment. To reduce the computational requirements, the nanotube surrounding the diamantane dicarboxylic acid has been represented by a cylindrical constraining potential. The dynamics has been accelerated by heating the system to T=1500 K. The molecular dynamics simulation of the entire process is shown as a movie in Supplementary Information.

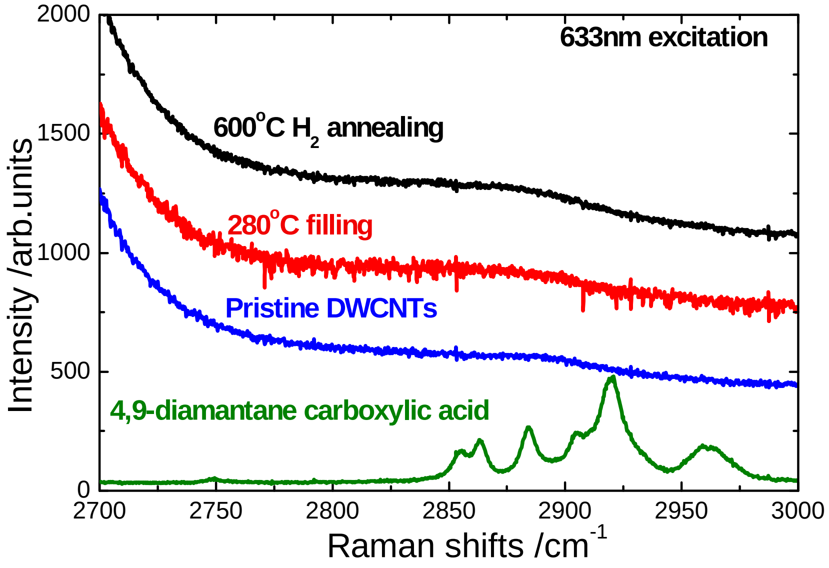

Figure S7. Raman spectra of 4,9-diamantane dicarboxylic acid encapsulation and annealing in DWCNTs as compared to pristine 4,9-diamantane dicarboxylic acid and DWCNTs.

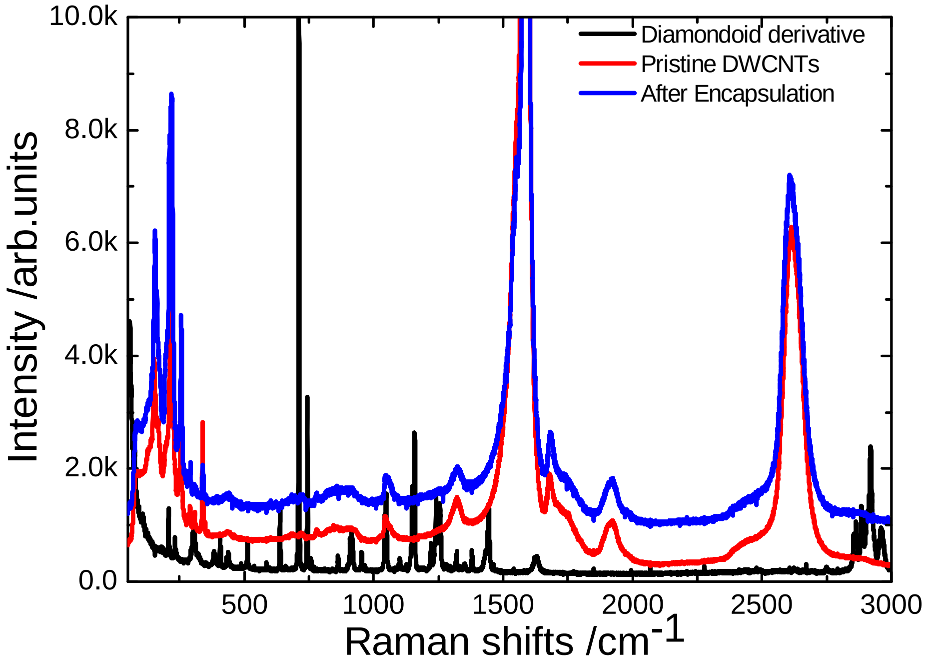

Figure S8. Raman spectra of 4,9-diamantane carboxylic acid (black), pristine DWCNTs (red) and diaacid@DWCNTs (blue), obtained using a 514 nm excitation.

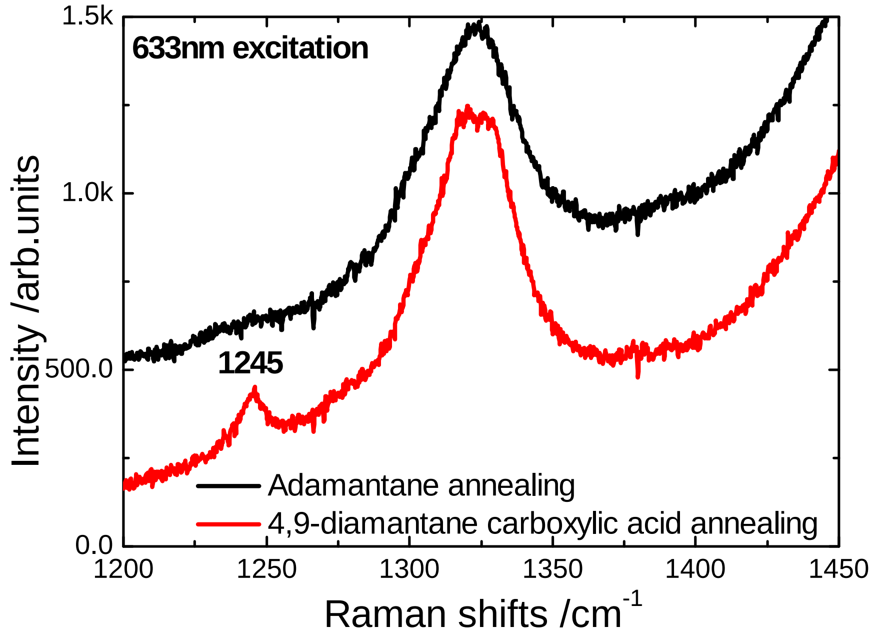

Figure S9. Raman spectra of the annealed samples of adamantane (black) and 4,9-diamantane carboxylic acid (red) in DWCNTs at 600°C under pure H_2 atmosphere.

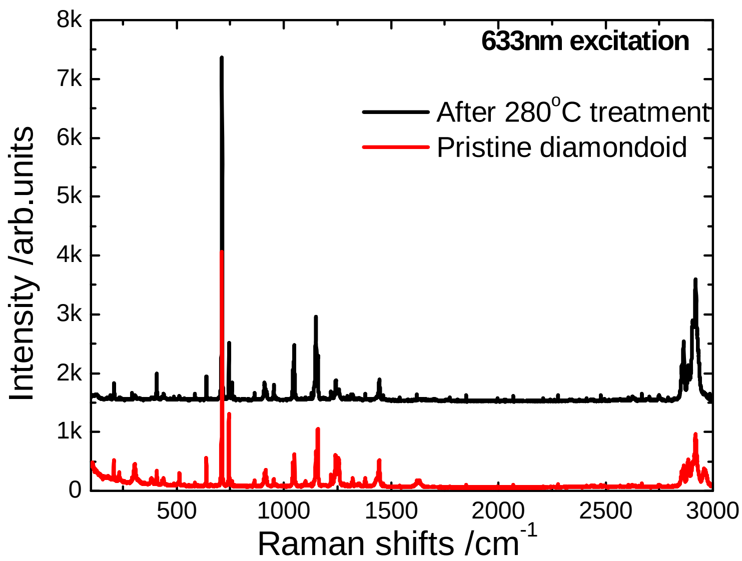

Figure S10. Raman spectra of 4,9-diamantane carboxylic acid before (red) and after (black) annealing at 280°C.

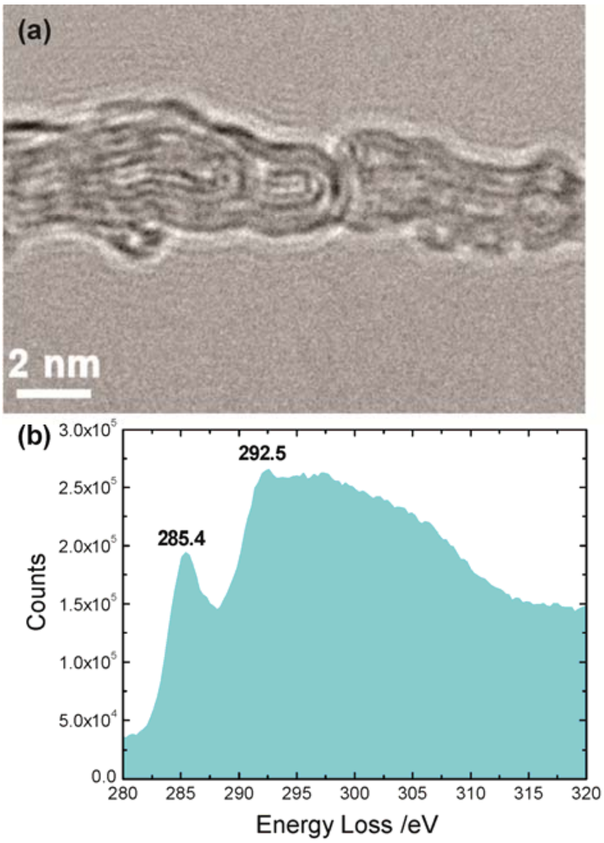

Figure S11. (a) HR-TEM image and (b) carbon K-edge absorption spectrum of filled DWCNTs following EELS measurements using intense electron beam irradiation.

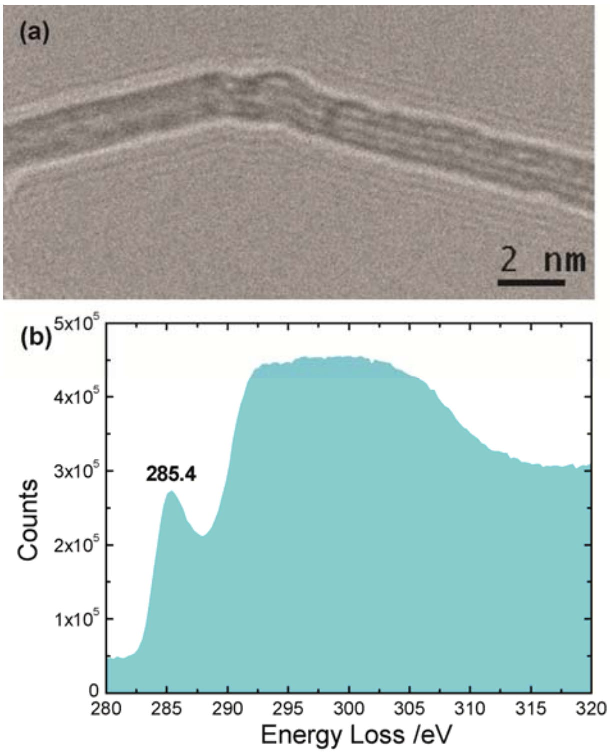

Figure S12. (a) HR-TEM image and (b) carbon K-edge absorption spectrum of empty DWCNTs following EELS measurements using intense electron beam irradiation.