Electronic Supplementary Material (ESI) for Nanoscale

Supplementary Information for

Multiple Intra-Tube Junctions in the Inner Walls of Peapods Derived DWNTs: Theoretical Study and Experimental Evidence

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Experimental Method

Synthesis, surface modification and characterizations of peapods-grown DWNTs: Highly purified arc-produced SWNTs (Hanwha Company, Korea) were used without further treatment. The SWNTs exhibit a diameter of about 1.3 - 1.4 nm and are used as the hosting fullerene material. After vaporizing fullerenes in a vacuum-sealed glass ampoule containing SWNTs at 600°C for 24 hrs, the reactants were washed twice in order to remove the residual fullerenes attached to the sidewall of the bundled SWNTs. Subsequently, the black paper-like peapods were dried under vacuum at 100°C for 24 hrs. Finally, by subjecting the sample prepared via a high-temperature thermal treatment at 1700 and 1800°C in an argon atmosphere using a graphite furnace, high-purity peapod-derived DWNTs were obtained.

The high resolution transmission electron microscopy (HRTEM) images were obtained using double CS corrector (CEOS GmbH) equipped JEM-2100F (80 kV, JEOL, Japan)

Table S1: The statistics of final tubes obtained by the coalescence of C_{120} tube + C_{60}:

Type of the C_{120} short tube			(9,0)	(10,0)	(6,3)	(6,5)	(5,5)
# of successful EDKMC runs			36	22	24	39	36
Chiral index	Diameter (nm)	Chiral angle					
(6, 3)	0.621	19.11 ^{o}			3		
(6, 5)	0.747	26.99 ^{o}				17	1
(5, 5)	0.678	30^o				7	30
(9, 0)	0.705	0 ^{o}	14				
(6, 4)	0.683	23.41 ^{o}	6		10	11	5
(7, 4)	0.755	21.05 ^{o}				4	
(7, 3)	0.696	17.00 ^{o}	8		11		
(9, 1)	0.747	5.21 ^{o}		5			
(8, 1)	0.669	5.82 ^{o}					
(8, 3)	0.771	15.29 ^{o}					
(6, 3)	0.621	19.11 ^{o}	8	17			

Table S2: The statistics of final tubes obtained by the coalescence of C_{180} tube + C_{60}:

Type of the C_{180} short tube			(8,4)	(7,3)	(9,0)	(6,5)
# of successful EDKMC runs			32	36	45	35
Chiral indexes	Diameter (nm)	Chiral angle				
(6, 3)	0.621	19.11 ^{o}				
(6, 5)	0.747	26.99 ^{o}	4			35
(5, 5)	0.678	30^{o}				
(9, 0)	0.705	0 ^{o}			45	
(6, 4)	0.683	23.41 ^{o}				
(7, 4)	0.755	21.05 ^{o}	5			
(7, 3)	0.696	17.00 ^{o}	6	36		
(8, 3)	0.771	15.29 ^{o}	5			
(8, 2)	0.718	10.89 ^{o}	12			