Supplementary Material (ESI) for Chemical Communications

Supporting information

Host-Guest Interactions in Azafullerene ($C_{59}N$)−Single−Wall Carbon Nanotubes (SWCNT) Peapod Hybrid Structures

Yoko Iizumi,[a, b] Toshiya Okazaki,[*, a, b, c] Zhen Liu, [b] Kazu Suenaga,[b] Takeshi Nakanishi,[b] Sumio Iijima,[b] Georgios Rotas,[d] and Nikos Tagmatarchis[d]

Department of Chemistry, University of Tsukuba, Tsukuba 305-8577, Japan, Nanotube Research Center, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba 305-8565, Japan, PRESTO, Japan Science and Technology Agency (JST), 4-1-8 Honcho, Kawaguchi 332-0012, Japan, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, 11635 Athens, Greece

Table S1. Observed optical transition energies of azafullerene NPDs in micelle solution.

	(*n*, *m*)	E_{11} (eV)	E_{22} (eV)
Type I	(13, 5)	0.842	1.255
	(12, 7)	0.783	1.308
	(11, 9)	0.750	1.300
	(16, 2)	0.775	1.246
	(15, 4)	0.752	1.248
	(14, 6)	0.735	1.249
	(13, 8)	0.714	1.232
	(12, 10)	0.691	1.196
Type II	(13, 6)	0.742	1.391
	(12, 8)	0.740	1.330
	(11, 10)	0.717	1.269
	(16, 3)	0.716	1.347
	(15, 5)	0.715	1.312
	(14, 7)	0.699	1.271
	(13, 9)	0.682	1.224

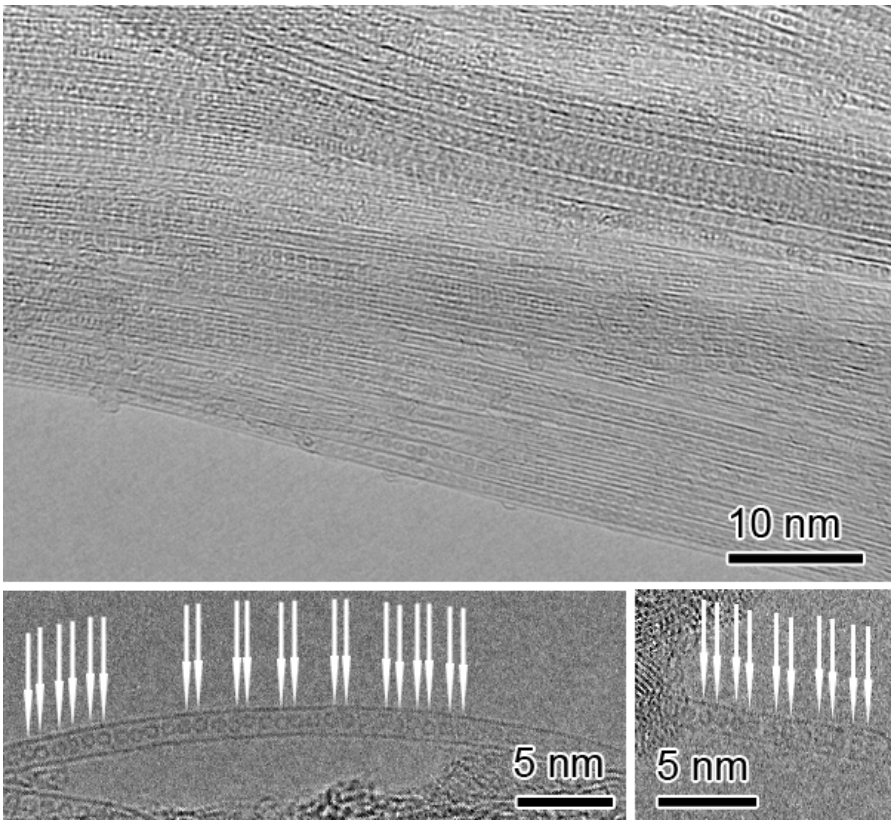

Figure S1. HR-TEM images of azafullerene NPDs. Azafullerene NPDs were produced in a high-yield. Arrows show the azafullerene dimer in SWCNTs, while some monomer and oligomer are also present. Azafullerenes were encapsulated in purified SWCNTs produced by the arc-discharging method (Meijo Arc APJ-type, Meijo Nano Carbon, Ltd.).

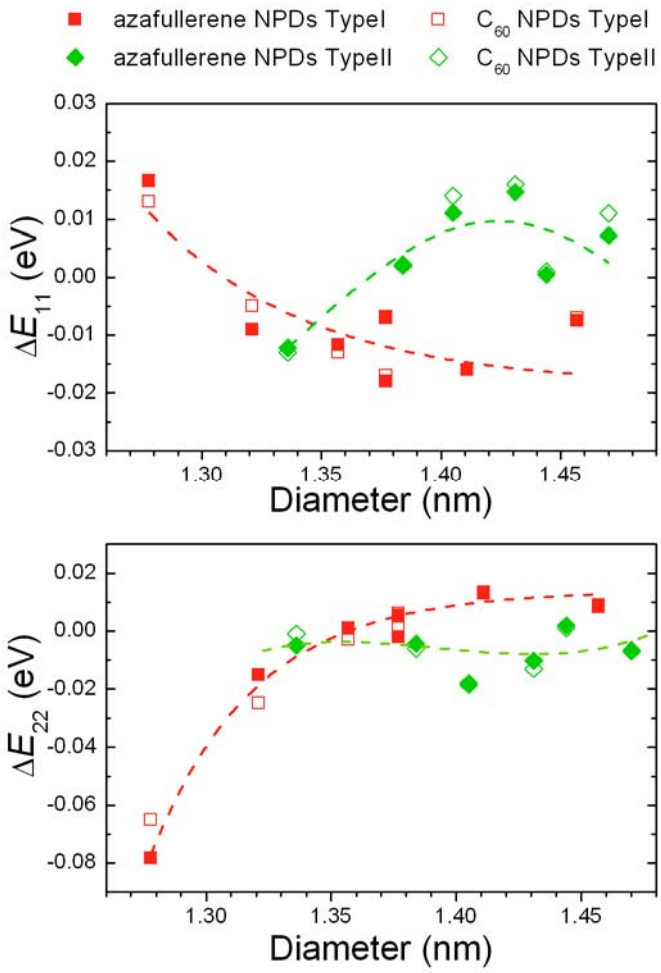

Figure S2. Differences in optical transition energy in E_{11} and E_{22} between azafullerene peapods and SWCNTs ($\Delta E_{ii} = E_{ii}^{NPDs} - E_{ii}^{SWCNTs}$, i = 1, 2) as a function of tube diameter, together with reference results of those of C_{60} NPDs.[10,11]