Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Carbon nanotube and boron nitride nanotube hosted C_{60}-V nanopeapods

Guiling Zhang,[1,3] Rulong Zhou,[2,3] Xiao Cheng Zeng[3,*]

[1]*Key Laboratory of Green Chemical Engineering and Technology of College of Heilongjiang Province, College of Chemical and Environmental Engineering, Harbin University of Science and Technology, Harbin 150040, China*

[2]*School of Science and Engineering of Materials, Hefei University of Technology, Hefei, Anhui, 230009, China*

[3]*Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588*

Table S1. Calculation Results Per Supercell of **1a**-**1h** and **2a**-**2h** Peapods in the Antiferromagnetic (AFM) and Ferromagnetic (FM) States: Total energy (E), Energy Difference between the FM and AFM States ($\Delta E_{FM\text{-}AFM}$), Total Magnetic Moment (S), and Reaction Energy (ΔE_r). The Data for V-free C_{60}@CNT and C_{60}@BNNT are Listed for Comparison. Abbreviation: hfh refers to hexagon-facing-haxagon, and pfh refers to pentagon-facing-hexagon.

Peapods	E_{AFM} (eV)	E_{FM} (eV)	$\Delta E_{FM\text{-}AFM}$ (meV)	S_{AFM}/S_{FM} (μ_B)	$\Delta E_{r,AFM}/\Delta E_{r,FM}$ (eV)
SIESTA Calculation Results					
Multi-Pod Structures					
1a (η^6-$C_{60}V$)@CNT	-68839.00998	-68838.90292	107.06	0.0/2.0	-18.54/-18.44
2a (η^6-$C_{60}V$)@BNNT	-77230.88150	-77230.80118	80.32	0.0/2.2	-18.44/-18.36
1b (η^5-$C_{60}H_{10}V$)@CNT	-69170.70640	-69170.70278	3.62	0.0/6.0	-26.68/-26.68
2b (η^5-$C_{60}H_{10}V$)@BNNT	-77562.45878	-77562.45640	2.38	0.0/6.0	-26.46/-26.46
1c (η^5-$C_{60}V$)@CNT	-68837.31546	-68837.13664	178.82	0.0/6.8	-16.86/-16.68
2c (η^5-$C_{60}V$)@BNNT	-77229.69066	-77229.38332	307.34	0.0/6.8	-17.26/-16.94
1d (η^6-$C_{60}H_{12}V$)@CNT	-69227.52458	-69227.50888	15.7	0.0/2.0	-21.22/-21.20
2d (η^6-$C_{60}H_{12}V$)@BNNT	-77618.17744	-77618.16876	8.68	0.0/2.0	-19.90/-19.88
V-Side-Binding Structures					
1e ($C_{60}V$)@CNT(hfh) *cis*	-68837.85062	-68837.93756	86.94	0.0/2.0	-
2e ($C_{60}V$)@BNNT(hfh) *cis*	-77228.04736	-77228.07838	31.02	0.0/2.0	-
1f ($C_{60}V$)@CNT(hfh) *trans*	-68837.94528	-68837.97022	24.94	0.0/2.0	-
2f ($C_{60}V$)@BNNT(hfh) *trans*	-77228.21776	-77228.19430	-23.46	0.0/2.0	-
1g ($C_{60}V$)@CNT(pfh) *cis*	-68837.65960	-68837.52740	-132.20	1.0/9.0	-
2g ($C_{60}V$)@BNNT(pfh) *cis*	-77227.83082	-77227.82054	-10.28	0.0/10.0	-
1h ($C_{60}V$)@CNT(pfh) *trans*	-68837.65586	-68837.65472	-1.14	0.0/10.0	-
2h ($C_{60}V$)@BNNT(pfh) *trans*	-77228.05754	-77228.04272	-14.82	0.0/10.0	-
V-free Species					
C_{60}@CNT (pfp)	-34056.85783	-	-	0.0	-6.92
C_{60}@CNT (hfh)	-34056.77958	-	-	0.0	-6.76
C_{60}@BNNT(pfp)	-38252.77402	-	-	0.0	-6.78
C_{60}@BNNT(hfh)	-38252.71239	-	-	0.0	-6.66
VASP Calculation Results					
1a (η^6-$C_{60}V$)@CNT	-4015.6230	-4015.5856	37.4	0.0/2.0	-
2a (η^6-$C_{60}V$)@BNNT	-3878.6422	-3878.5124	129.8	0.0/2.0	-
1b (η^5-$C_{60}H_{10}V$)@CNT	-4095.1300	-4095.1304	0.4	0.0/6.0	-
2b (η^5-$C_{60}H_{10}V$)@BNNT	-3958.8224	-3958.8206	1.8	0.0/6.0	-
1c (η^5-$C_{60}V$)@CNT	-4013.5262	-4013.4626	63.6	0.0/6.8	-
2c (η^5-$C_{60}V$)@BNNT	-3877.4412	-3877.2968	144.4	0.0/7.0	-
1d (η^6-$C_{60}H_{12}V$)@CNT	-4101.5286	-4101.4628	65.8	0.0/2.0	-
2d (η^6-$C_{60}H_{12}V$)@BNNT	-3964.2970	-3964.2896	7.4	0.0/2.0	-

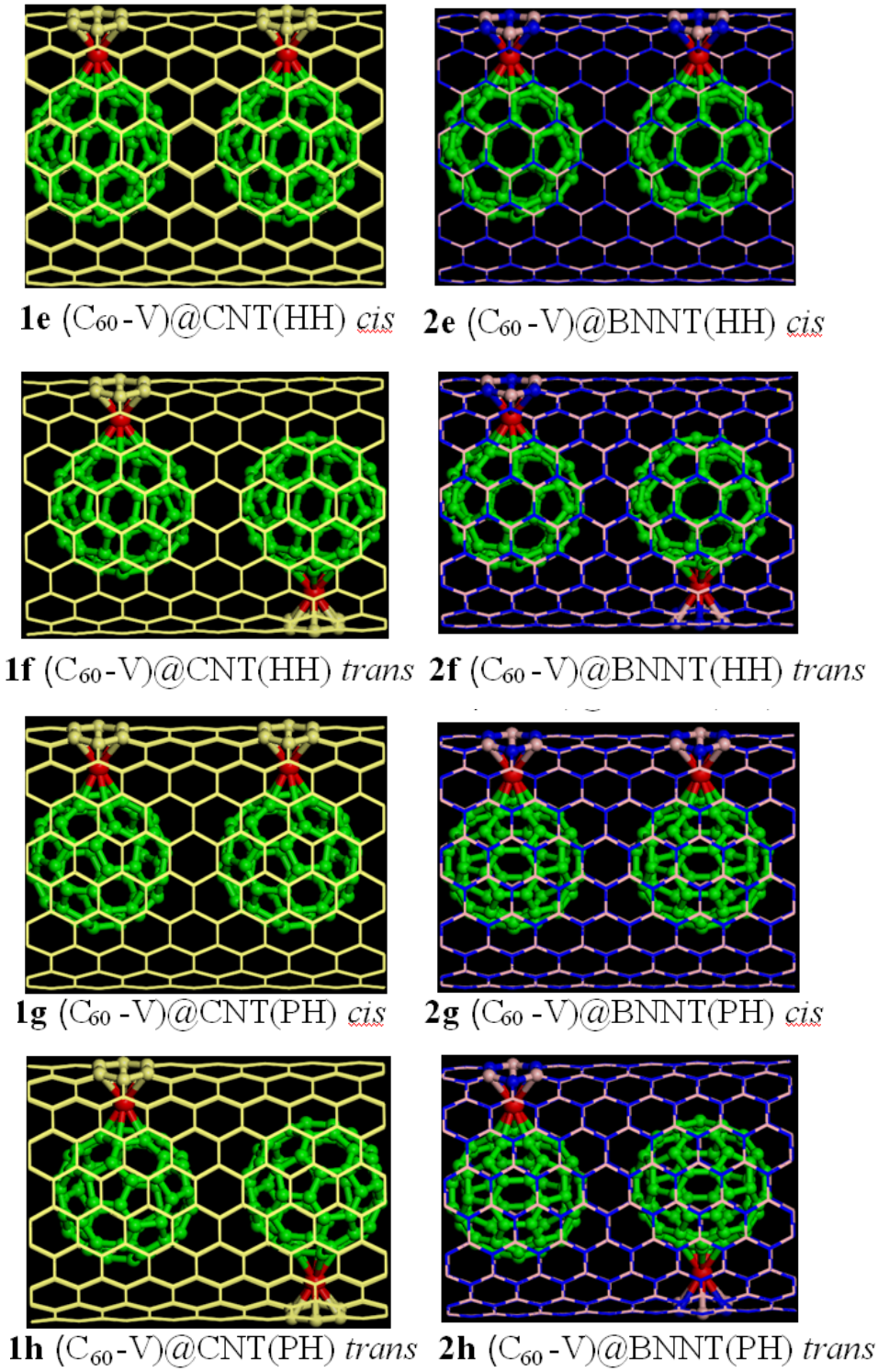

Figure S1. Optimized side-V-binding structures of **1e-1h** and **2e-2h** peapods. We denote a pVh structure if the C_{60} uses the pentagon and the tube uses the pentagon to coordinate with the V atom and a HH structure if both C_{60} and tube use the hexagon.

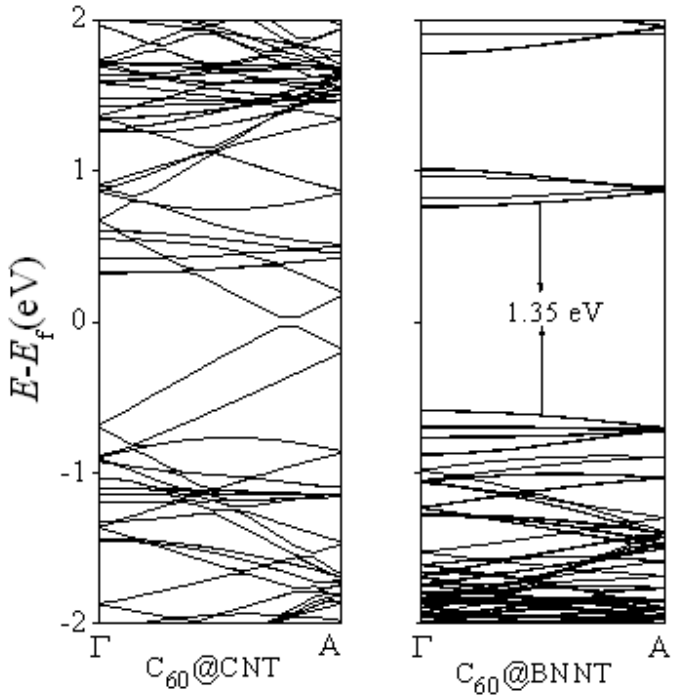

Figure S2. Computed band structures of C_{60}@CNT and C_{60}@BNNT peapods.