Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

DFT Investigation of Interactions between Single-Walled Carbon Nanotubes and Fluorene-Based Conjugated Oligomers

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Table S1. Selected bond lengths (R) (in Å), bond angles (A) (in degrees), and dihedral angles (D_h) (in degrees) of the isolated DPF-ALD without SCs. The labeling of atoms is shown in Figure 1.

Bond Length (R)	**B97D**	**wB97XD**	**CAM-B3LYP**	**B3LYP**
R_{1-2}	1.482	1.480	1.476	1.478
R_{2-3}	1.412	1.398	1.396	1.403
R_{3-4}	1.393	1.385	1.383	1.387
R_{4-5}	1.419	1.403	1.403	1.411
R_{5-6}	1.481	1.484	1.482	1.483
R_{6-7}	1.418	1.403	1.401	1.409
R_{7-8}	1.399	1.390	1.388	1.393
R_{8-9}	1.405	1.391	1.390	1.397
R_{9-10}	1.463	1.467	1.466	1.465
R_{10-11}	1.405	1.391	1.390	1.397
R_{11-12}	1.399	1.390	1.388	1.393
R_{12-13}	1.418	1.402	1.410	1.409
R_{13-14}	1.481	1.483	1.482	1.482
R_{14-15}	1.416	1.400	1.399	1.407
R_{15-16}	1.397	1.388	1.387	1.391
R_{16-17}	1.410	1.395	1.393	1.401
R_{17-18}	1.482	1.480	1.476	1.478
Bond Angle (A)				
A_{1-2-3}	120.9	120.4	120.3	120.6
A_{2-3-4}	120.2	120.0	120.1	120.2
A_{3-4-5}	121.0	120.8	120.9	121.1
A_{4-5-6}	120.9	120.6	120.8	120.9
A_{5-6-7}	120.6	120.3	120.5	120.6
A_{6-7-8}	121.6	121.3	121.4	121.6
A_{7-8-9}	119.0	118.9	119.0	119.1
A_{8-9-10}	131.1	131.2	131.3	131.4
$A_{9-10-11}$	131.1	131.2	131.3	131.4
$A_{10-11-12}$	118.9	118.3	119.0	119.1
$A_{11-12-13}$	121.6	121.3	121.5	121.6
$A_{12-13-14}$	120.6	120.4	120.5	120.7
$A_{13-14-15}$	120.9	120.7	120.8	120.9
$A_{14-15-16}$	120.7	120.6	120.7	120.8
$A_{15-16-17}$	120.5	120.3	120.3	120.5
$A_{16-17-18}$	119.8	120.0	120.2	120.2
Dihedral Angle (D_h)				
$D_{1-2-3-4}$	179.9	179.9	-180.0	180.0

Table S1 (continued):

$D_{2\text{-}3\text{-}4\text{-}5}$	0.1	-0.1	-0.1	0.1
$D_{3\text{-}4\text{-}5\text{-}6}$	-179.9	-179.7	-180.0	179.9
$D_{4\text{-}5\text{-}6\text{-}7}$	-33.5	41.2	38.3	36.4
$D_{5\text{-}6\text{-}7\text{-}8}$	-180.0	180.0	179.9	179.9
$D_{6\text{-}7\text{-}8\text{-}9}$	-0.1	0.1	0.1	0.2
$D_{7\text{-}8\text{-}9\text{-}10}$	-179.6	179.6	179.8	179.7
$D_{8\text{-}9\text{-}10\text{-}11}$	0.0	0.1	0.5	0.6
$D_{9\text{-}10\text{-}11\text{-}12}$	179.6	-179.7	179.8	179.7
$D_{10\text{-}11\text{-}12\text{-}13}$	0.1	-0.1	0.1	0.2
$D_{11\text{-}12\text{-}13\text{-}14}$	-179.9	180.0	-180.0	180.0
$D_{12\text{-}13\text{-}14\text{-}15}$	33.6	-41.4	38.3	36.6
$D_{13\text{-}14\text{-}15\text{-}16}$	179.9	-180.0	180.0	179.9
$D_{14\text{-}15\text{-}16\text{-}17}$	-0.1	0.1	-0.1	0.1
$D_{15\text{-}16\text{-}17\text{-}18}$	-179.9	179.9	-179.9	179.9

Table S2. Selected bond lengths (R) (in Å), bond angles (A) (in degrees), and dihedral angles (D_h) (in degrees) of the isolated DPF-DTF without SCs. The labeling of atoms is shown in Figure 1.

Bond Length (R)	**B97D**	**wB97XD**	**CAM-B3LYP**	**B3LYP**
R_{1-2}	1.457	1.465	1.462	1.458
R_{2-3}	1.419	1.402	1.401	1.410
R_{3-4}	1.396	1.389	1.387	1.391
R_{4-5}	1.414	1.398	1.397	1.405
R_{5-6}	1.480	1.483	1.482	1.481
R_{6-7}	1.418	1.403	1.402	1.410
R_{7-8}	1.399	1.390	1.389	1.393
R_{8-9}	1.405	1.391	1.389	1.397
R_{9-10}	1.463	1.468	1.467	1.466
R_{10-11}	1.405	1.391	1.389	1.397
R_{11-12}	1.399	1.390	1.386	1.393
R_{12-13}	1.418	1.402	1.402	1.409
R_{13-14}	1.480	1.482	1.482	1.481
R_{14-15}	1.416	1.400	1.399	1.407
R_{15-16}	1.393	1.385	1.383	1.387
R_{16-17}	1.422	1.404	1.403	1.412
R_{17-18}	1.457	1.464	1.462	1.458
Bond Angle (A)				
A_{1-2-3}	125.6	124.2	124.9	125.5
A_{2-3-4}	121.2	121.0	121.1	121.3
A_{3-4-5}	121.8	121.3	121.5	121.8
A_{4-5-6}	121.4	121.1	121.3	121.5
A_{5-6-7}	120.7	120.4	120.6	120.8
A_{6-7-8}	121.7	121.4	121.5	121.7
A_{7-8-9}	119.0	118.9	119.0	119.2
A_{8-9-10}	131.3	131.2	131.4	131.5
$A_{9-10-11}$	131.3	131.2	131.4	131.5
$A_{10-11-12}$	119.0	118.9	119.1	119.2
$A_{11-12-13}$	121.7	121.4	121.5	121.7
$A_{12-13-14}$	120.8	120.5	120.7	120.8
$A_{13-14-15}$	121.5	121.2	121.3	121.5
$A_{14-15-16}$	121.2	120.9	121.1	121.2
$A_{15-16-17}$	121.8	121.5	121.6	121.9
$A_{16-17-18}$	117.6	118.1	118.0	117.8
Dihedral Angle (D_h)				
$D_{1-2-3-4}$	179.3	179.3	179.6	179.6

Table S2 (continued):

$D_{2\text{-}3\text{-}4\text{-}5}$	0.3	0.5	0.3	0.2
$D_{3\text{-}4\text{-}5\text{-}6}$	-179.8	180.0	-179.9	179.9
$D_{4\text{-}5\text{-}6\text{-}7}$	32.6	41.7	38.1	36.0
$D_{5\text{-}6\text{-}7\text{-}8}$	-179.8	-179.7	-179.9	180.0
$D_{6\text{-}7\text{-}8\text{-}9}$	-0.1	0.0	-0.1	0.1
$D_{7\text{-}8\text{-}9\text{-}10}$	179.7	179.6	179.8	179.8
$D_{8\text{-}9\text{-}10\text{-}11}$	0.7	1.2	0.6	0.6
$D_{9\text{-}10\text{-}11\text{-}12}$	180.0	179.9	179.9	179.9
$D_{10\text{-}11\text{-}12\text{-}13}$	-0.1	0.1	0.1	0.1
$D_{11\text{-}12\text{-}13\text{-}14}$	179.9	179.7	180.0	180.0
$D_{12\text{-}13\text{-}14\text{-}15}$	32.0	41.9	37.6	35.5
$D_{13\text{-}14\text{-}15\text{-}16}$	179.9	180.0	179.9	179.8
$D_{14\text{-}15\text{-}16\text{-}17}$	-0.5	-0.4	-0.5	0.4
$D_{15\text{-}16\text{-}17\text{-}18}$	-179.3	-179.8	-179.4	179.4

Table S3. Selected bond lengths (R) (in Å), bond angles (A) (in degrees), and dihedral angles (D_h) (in degrees) of the isolated DPF-ALD with 2 SCs. The labeling of atoms is shown in Figure 1.

Bond Length (R)	**B97D**	**wB97XD**	**CAM-B3LYP**	**B3LYP**
R_{1-2}	1.481	1.480	1.477	1.478
R_{2-3}	1.412	1.398	1.396	1.404
R_{3-4}	1.393	1.385	1.383	1.387
R_{4-5}	1.419	1.403	1.403	1.411
R_{5-6}	1.481	1.483	1.482	1.483
R_{6-7}	1.418	1.402	1.401	1.409
R_{7-8}	1.399	1.391	1.389	1.393
R_{8-9}	1.404	1.390	1.389	1.396
R_{9-10}	1.463	1.468	1.466	1.465
R_{10-11}	1.404	1.390	1.389	1.396
R_{11-12}	1.400	1.391	1.389	1.393
R_{12-13}	1.418	1.402	1.401	1.409
R_{13-14}	1.480	1.483	1.482	1.483
R_{14-15}	1.416	1.400	1.399	1.407
R_{15-16}	1.397	1.388	1.387	1.391
R_{16-17}	1.410	1.395	1.393	1.401
R_{17-18}	1.482	1.480	1.476	1.478
Bond Angle (A)				
A_{1-2-3}	120.9	120.3	120.3	120.6
A_{2-3-4}	120.2	120.1	120.1	120.2
A_{3-4-5}	121.0	120.8	120.9	121.1
A_{4-5-6}	121.0	120.8	120.8	121.0
A_{5-6-7}	120.6	120.5	120.4	120.6
A_{6-7-8}	121.5	121.3	121.3	121.5
A_{7-8-9}	118.9	118.9	119.0	119.1
A_{8-9-10}	131.5	131.4	131.2	131.3
$A_{9-10-11}$	131.5	131.3	131.3	131.3
$A_{10-11-12}$	118.9	118.9	119.0	119.1
$A_{11-12-13}$	121.6	121.3	121.4	121.5
$A_{12-13-14}$	120.7	120.6	120.6	120.7
$A_{13-14-15}$	121.0	120.6	120.8	120.9
$A_{14-15-16}$	120.7	120.5	120.7	120.8
$A_{15-16-17}$	120.5	120.3	120.3	120.5
$A_{16-17-18}$	119.9	120.0	120.3	120.2
Dihedral Angle (D_h)				
$D_{1-2-3-4}$	-179.9	180.0	179.9	180.0

Table S3 (continued):

$D_{2\text{-}3\text{-}4\text{-}5}$	-0.1	-0.2	-0.1	-0.1
$D_{3\text{-}4\text{-}5\text{-}6}$	-179.8	-179.8	-179.7	-179.7
$D_{4\text{-}5\text{-}6\text{-}7}$	33.6	40.8	38.9	37.0
$D_{5\text{-}6\text{-}7\text{-}8}$	179.1	179.4	179.7	179.4
$D_{6\text{-}7\text{-}8\text{-}9}$	0.1	-0.1	0.2	0.1
$D_{7\text{-}8\text{-}9\text{-}10}$	-179.6	-179.7	179.8	-179.9
$D_{8\text{-}9\text{-}10\text{-}11}$	-0.6	-1.2	0.2	-0.3
$D_{9\text{-}10\text{-}11\text{-}12}$	-179.6	-179.1	-179.9	-179.4
$D_{10\text{-}11\text{-}12\text{-}13}$	-0.2	-0.2	0.0	-0.1
$D_{11\text{-}12\text{-}13\text{-}14}$	179.9	179.4	180.0	179.6
$D_{12\text{-}13\text{-}14\text{-}15}$	-33.7	-41.6	-37.9	-36.5
$D_{13\text{-}14\text{-}15\text{-}16}$	-179.8	-179.5	180.0	-179.8
$D_{14\text{-}15\text{-}16\text{-}17}$	0.1	0.1	0.2	0.1
$D_{15\text{-}16\text{-}17\text{-}18}$	179.9	179.8	179.8	179.9

Table S4. Selected bond lengths (R) (in Å), bond angles (A) (in degrees), and dihedral angles (D_h) (in degrees) of the isolated DPF-ALD with 6 SCs. The labeling of atoms is shown in Figure 1.

Bond Length (R)	**B97D**	**wB97XD**	**CAM-B3LYP**	**B3LYP**
R_{1-2}	1.480	1.479	1.476	1.477
R_{2-3}	1.414	1.407	1.405	1.414
R_{3-4}	1.399	1.400	1.396	1.400
R_{4-5}	1.424	1.390	1.394	1.403
R_{5-6}	1.483	1.488	1.485	1.487
R_{6-7}	1.416	1.400	1.380	1.408
R_{7-8}	1.404	1.394	1.390	1.394
R_{8-9}	1.406	1.390	1.388	1.396
R_{9-10}	1.470	1.469	1.467	1.465
R_{10-11}	1.404	1.391	1.390	1.396
R_{11-12}	1.406	1.390	1.389	1.393
R_{12-13}	1.412	1.400	1.401	1.409
R_{13-14}	1.485	1.486	1.485	1.486
R_{14-15}	1.404	1.409	1.408	1.417
R_{15-16}	1.409	1.387	1.386	1.392
R_{16-17}	1.421	1.403	1.398	1.405
R_{17-18}	1.482	1.480	1.476	1.477
Bond Angle (A)				
A_{1-2-3}	118.8	124.0	124.2	124.5
A_{2-3-4}	122.0	118.7	118.6	118.6
A_{3-4-5}	119.2	121.3	122.2	122.6
A_{4-5-6}	124.9	121.8	119.2	118.8
A_{5-6-7}	122.9	121.6	119.7	119.5
A_{6-7-8}	121.1	120.8	121.4	121.6
A_{7-8-9}	119.3	118.9	118.9	119.0
A_{8-9-10}	132.3	131.5	131.2	131.3
$A_{9-10-11}$	132.1	131.2	131.3	131.3
$A_{10-11-12}$	119.0	118.9	119.2	119.4
$A_{11-12-13}$	121.1	121.0	121.2	121.3
$A_{12-13-14}$	122.2	120.9	121.7	121.8
$A_{13-14-15}$	121.0	119.5	122.5	122.8
$A_{14-15-16}$	121.3	119.7	119.2	119.2
$A_{15-16-17}$	119.1	121.2	122.2	122.4
$A_{16-17-18}$	122.1	116.8	116.7	116.7
Dihedral Angle (D_h)				
$D_{1-2-3-4}$	-179.8	-178.7	-179.9	179.9

Table S4 (continued):

$D_{2\text{-}3\text{-}4\text{-}5}$	-0.5	-0.5	0.1	0.5
$D_{3\text{-}4\text{-}5\text{-}6}$	-179.4	176.7	-179.4	179.5
$D_{4\text{-}5\text{-}6\text{-}7}$	-48.0	76.3	47.4	44.6
$D_{5\text{-}6\text{-}7\text{-}8}$	-166.4	173.1	-178.4	177.0
$D_{6\text{-}7\text{-}8\text{-}9}$	-0.4	0.0	0.5	0.5
$D_{7\text{-}8\text{-}9\text{-}10}$	169.7	-176.0	179.9	179.0
$D_{8\text{-}9\text{-}10\text{-}11}$	0.4	-4.4	0.9	0.8
$D_{9\text{-}10\text{-}11\text{-}12}$	-170.5	-176.7	179.3	179.7
$D_{10\text{-}11\text{-}12\text{-}13}$	0.5	-1.4	0.3	0.3
$D_{11\text{-}12\text{-}13\text{-}14}$	173.3	175.9	177.9	177.6
$D_{12\text{-}13\text{-}14\text{-}15}$	58.5	-63.3	45.6	44.0
$D_{13\text{-}14\text{-}15\text{-}16}$	175.7	-176.4	178.6	179.2
$D_{14\text{-}15\text{-}16\text{-}17}$	-0.7	-1.0	0.1	0.3
$D_{15\text{-}16\text{-}17\text{-}18}$	-177.7	179.7	180.0	180.0

Table S5. Selected bond lengths (R) (in Å), bond angles (A) (in degrees), and dihedral angles (D_h) (in degrees) of the isolated DPF-DTF with 6 SCs. The labeling of atoms is shown in Figure 1.

Bond Length (R)	**B97D**	**wB97XD**	**CAM-B3LYP**	**B3LYP**
R_{1-2}	1.458	1.466	1.463	1.460
R_{2-3}	1.418	1.401	1.400	1.408
R_{3-4}	1.396	1.389	1.387	1.390
R_{4-5}	1.414	1.398	1.397	1.405
R_{5-6}	1.480	1.483	1.481	1.482
R_{6-7}	1.418	1.402	1.401	1.409
R_{7-8}	1.400	1.391	1.389	1.393
R_{8-9}	1.404	1.390	1.389	1.396
R_{9-10}	1.463	1.467	1.466	1.465
R_{10-11}	1.404	1.390	1.389	1.397
R_{11-12}	1.400	1.391	1.389	1.394
R_{12-13}	1.418	1.402	1.401	1.409
R_{13-14}	1.480	1.483	1.482	1.482
R_{14-15}	1.416	1.401	1.400	1.407
R_{15-16}	1.394	1.386	1.384	1.388
R_{16-17}	1.421	1.403	1.402	1.411
R_{17-18}	1.457	1.466	1.464	1.460
Bond Angle (A)				
A_{1-2-3}	124.7	123.6	123.8	124.3
A_{2-3-4}	121.2	121.0	121.1	121.2
A_{3-4-5}	121.7	121.2	121.4	121.6
A_{4-5-6}	121.3	121.1	121.1	121.2
A_{5-6-7}	120.6	120.6	120.4	120.5
A_{6-7-8}	121.7	121.4	121.5	121.6
A_{7-8-9}	119.0	119.0	119.1	119.2
A_{8-9-10}	131.5	131.4	131.3	131.3
$A_{9-10-11}$	131.6	131.4	131.3	131.5
$A_{10-11-12}$	119.0	118.9	119.1	119.2
$A_{11-12-13}$	121.7	121.4	121.5	121.6
$A_{12-13-14}$	120.9	120.6	120.5	121.0
$A_{13-14-15}$	121.9	121.6	121.5	122.1
$A_{14-15-16}$	121.2	121.0	121.1	121.2
$A_{15-16-17}$	121.7	121.3	121.5	121.7
$A_{16-17-18}$	118.2	118.9	118.6	118.9
Dihedral Angle (D_h)				
$D_{1-2-3-4}$	177.6	179.2	178.3	176.9

Table S5 (continued):

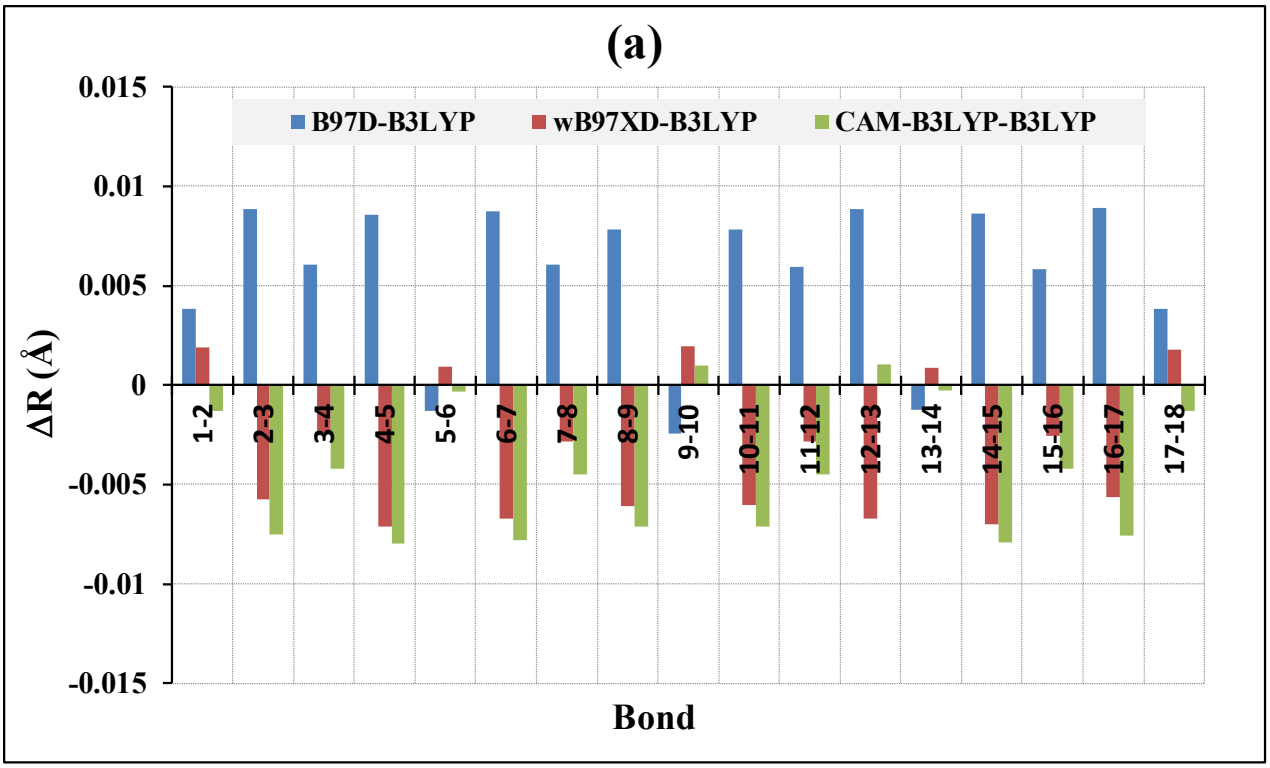
$D_{2\text{-}3\text{-}4\text{-}5}$	0.5	0.4	0.4	0.4
$D_{3\text{-}4\text{-}5\text{-}6}$	-179.4	179.8	-179.1	-178.9
$D_{4\text{-}5\text{-}6\text{-}7}$	31.3	39.8	36.6	33.9
$D_{5\text{-}6\text{-}7\text{-}8}$	-179.5	-179.6	-179.8	-179.2
$D_{6\text{-}7\text{-}8\text{-}9}$	-0.2	-0.2	-0.2	-0.3
$D_{7\text{-}8\text{-}9\text{-}10}$	178.8	179.3	179.3	178.2
$D_{8\text{-}9\text{-}10\text{-}11}$	-0.9	-0.4	-0.3	-0.8
$D_{9\text{-}10\text{-}11\text{-}12}$	-177.0	-178.0	-178.4	-176.4
$D_{10\text{-}11\text{-}12\text{-}13}$	-0.3	-0.2	-0.2	-0.4
$D_{11\text{-}12\text{-}13\text{-}14}$	177.0	177.4	178.0	176.2
$D_{12\text{-}13\text{-}14\text{-}15}$	31.1	39.7	36.5	33.9
$D_{13\text{-}14\text{-}15\text{-}16}$	-178.2	-178.4	-178.3	-178.0
$D_{14\text{-}15\text{-}16\text{-}17}$	-0.7	-0.6	-0.7	-0.7
$D_{15\text{-}16\text{-}17\text{-}18}$	-179.9	179.8	179.6	-179.9

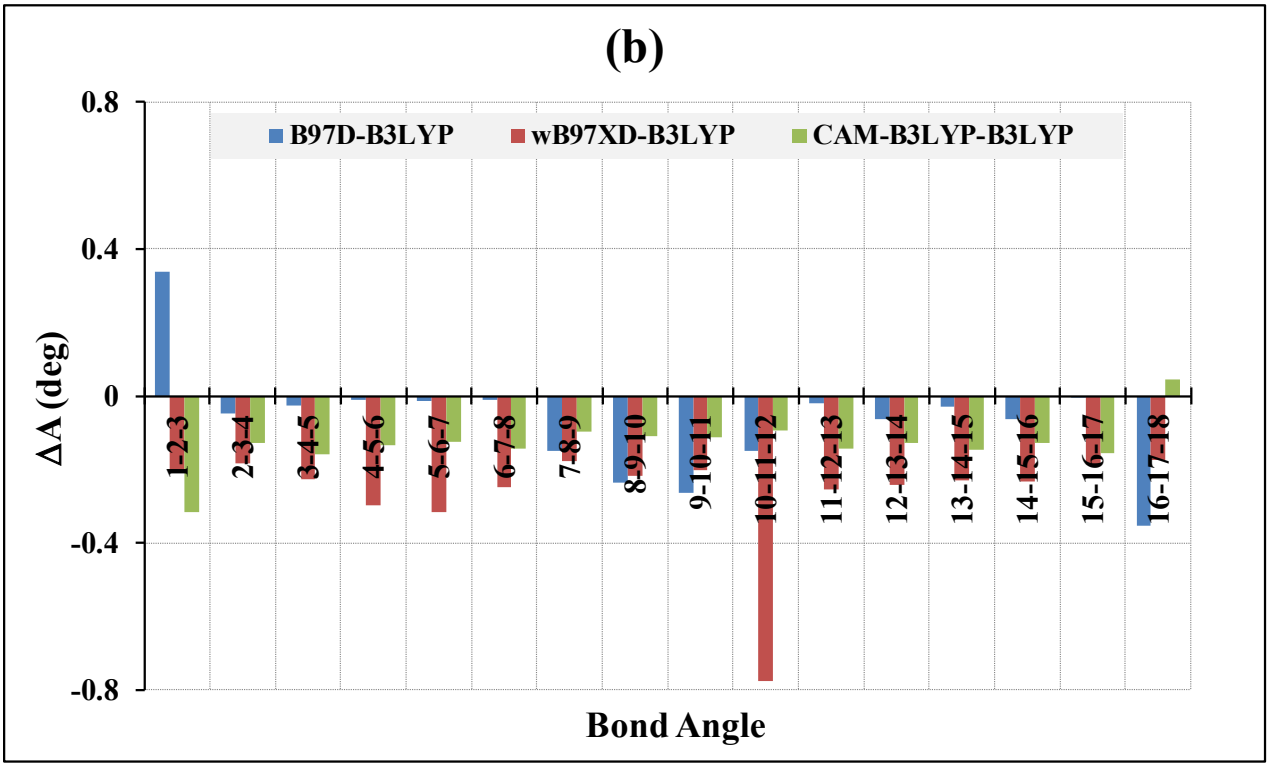
Table S6. Selected bond lengths (R) (in Å), bond angles (A) (in degrees), and dihedral angles (D_h) (in degrees) of the isolated DPF-DTF with 10 SCs. The labeling of atoms is shown in Figure 1.

Bond Length (R)	**B97D**	**wB97XD**	**CAM-B3LYP**	**B3LYP**
R_{1-2}	1.465	1.470	1.468	1.466
R_{2-3}	1.422	1.403	1.402	1.411
R_{3-4}	1.404	1.395	1.393	1.397
R_{4-5}	1.409	1.393	1.394	1.403
R_{5-6}	1.483	1.484	1.485	1.486
R_{6-7}	1.416	1.400	1.400	1.409
R_{7-8}	1.402	1.392	1.390	1.394
R_{8-9}	1.404	1.389	1.388	1.396
R_{9-10}	1.465	1.468	1.468	1.465
R_{10-11}	1.405	1.391	1.390	1.397
R_{11-12}	1.401	1.390	1.389	1.393
R_{12-13}	1.417	1.402	1.400	1.409
R_{13-14}	1.483	1.484	1.485	1.486
R_{14-15}	1.420	1.404	1.405	1.414
R_{15-16}	1.402	1.391	1.389	1.393
R_{16-17}	1.418	1.403	1.401	1.409
R_{17-18}	1.463	1.469	1.467	1.465
Bond Angle (A)				
A_{1-2-3}	125.0	123.7	124.2	125.1
A_{2-3-4}	119.9	119.8	119.8	119.8
A_{3-4-5}	122.3	121.7	122.2	122.7
A_{4-5-6}	119.9	120.2	119.5	119.1
A_{5-6-7}	119.8	120.1	119.8	119.5
A_{6-7-8}	121.6	121.3	121.5	121.8
A_{7-8-9}	118.9	118.8	119.0	119.1
A_{8-9-10}	131.7	131.4	131.4	131.4
$A_{9-10-11}$	131.9	131.5	131.5	131.4
$A_{10-11-12}$	119.2	119.1	119.3	119.4
$A_{11-12-13}$	121.2	121.0	121.2	121.4
$A_{12-13-14}$	122.2	121.5	121.9	121.9
$A_{13-14-15}$	124.8	124.0	123.5	123.1
$A_{14-15-16}$	119.6	119.4	119.6	119.7
$A_{15-16-17}$	122.7	122.2	122.4	122.7
$A_{16-17-18}$	117.6	118.0	117.7	117.2
Dihedral Angle (D_h)				
$D_{1-2-3-4}$	177.2	178.6	-179.9	179.4

Table S6 (continued):

$D_{2\text{-}3\text{-}4\text{-}5}$	2.1	1.7	1.3	1.6
$D_{3\text{-}4\text{-}5\text{-}6}$	-177.8	-179.4	180.0	179.1
$D_{4\text{-}5\text{-}6\text{-}7}$	44.2	51.5	45.6	41.6
$D_{5\text{-}6\text{-}7\text{-}8}$	178.0	179.3	-177.9	177.5
$D_{6\text{-}7\text{-}8\text{-}9}$	0.2	0.2	0.2	0.1
$D_{7\text{-}8\text{-}9\text{-}10}$	-179.0	179.7	179.1	179.7
$D_{8\text{-}9\text{-}10\text{-}11}$	-1.1	-1.3	0.1	0.7
$D_{9\text{-}10\text{-}11\text{-}12}$	-175.5	-174.4	-177.6	179.7
$D_{10\text{-}11\text{-}12\text{-}13}$	0.5	0.2	0.4	0.4
$D_{11\text{-}12\text{-}13\text{-}14}$	169.4	168.6	173.8	177.5
$D_{12\text{-}13\text{-}14\text{-}15}$	47.0	52.4	48.4	46.0
$D_{13\text{-}14\text{-}15\text{-}16}$	-179.9	-178.1	179.2	178.1
$D_{14\text{-}15\text{-}16\text{-}17}$	0.7	-0.2	0.0	0.1
$D_{15\text{-}16\text{-}17\text{-}18}$	-179.8	178.5	-179.9	179.4


(a)
B97D-B3LYP
wB97XD-B3LYP
CAM-B3LYP-B3LYP
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D-B3LYP
wB97XD-B3LYP
CAM-B3LYP-B3LYP
0.8
0.4
0
-0.4
-0.8
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

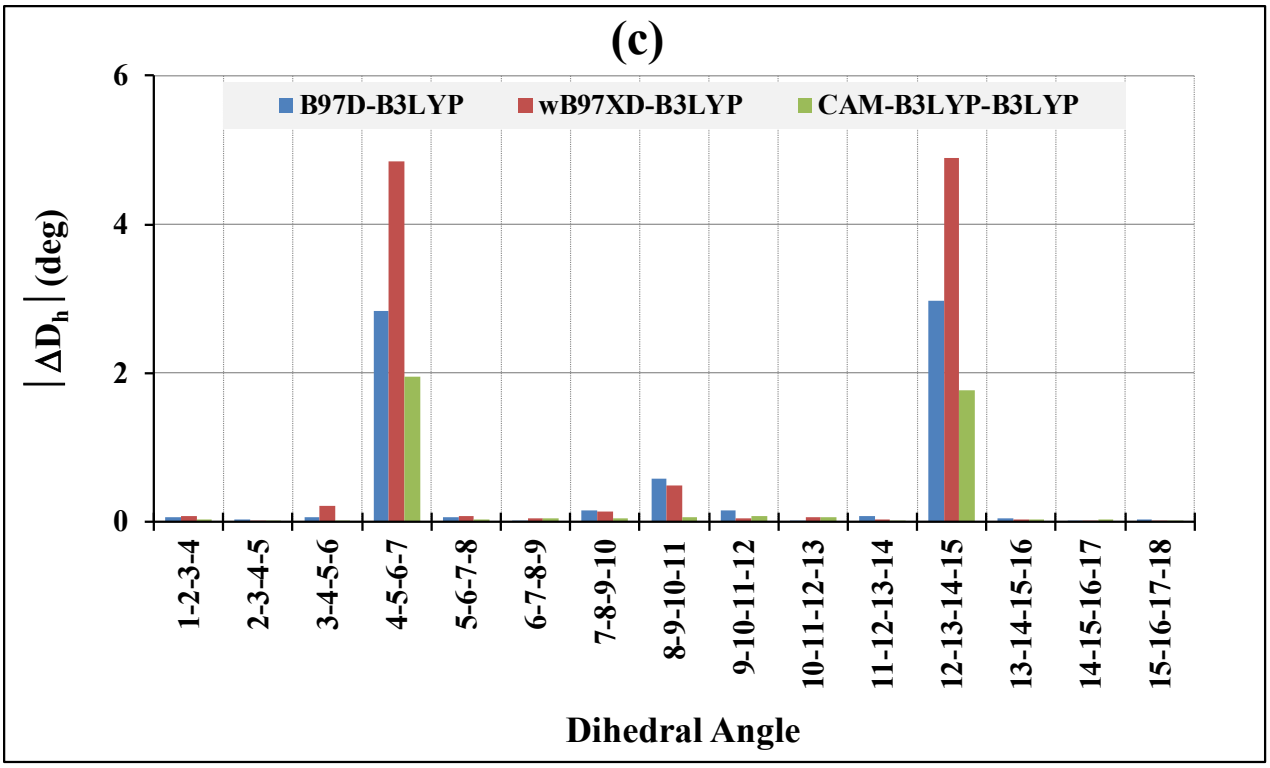
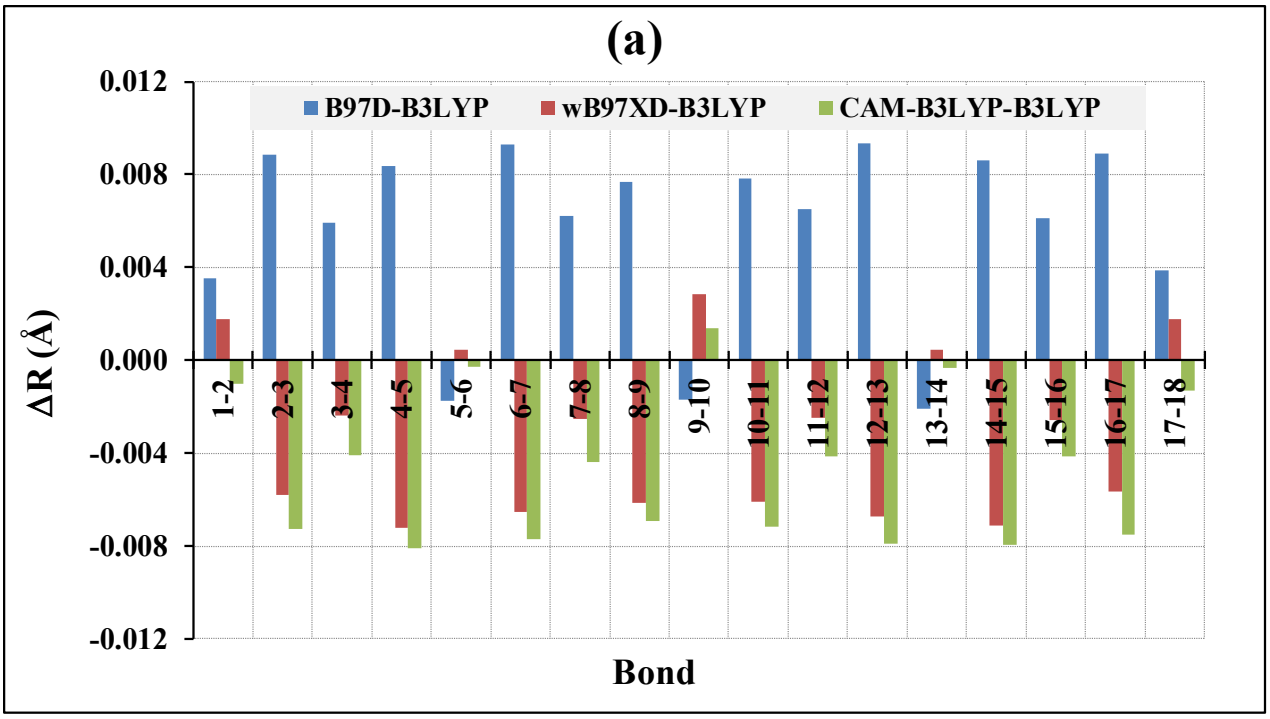
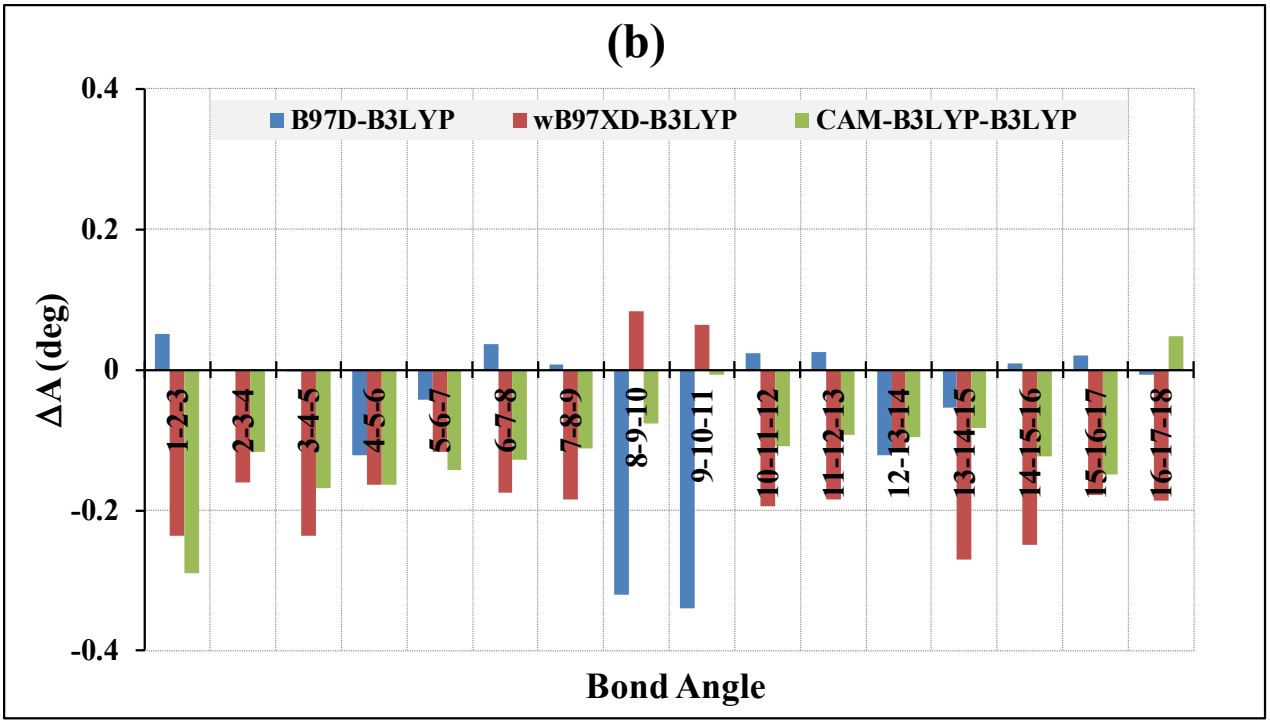


Figure S1. DFT method effect; comparison of the B3LYP geometrical parameters with other DFT methods' results for the isolated DPF-ALD without SCs. The labeling of atoms is shown in Figure 1. This figure shows differences between (a) bond lengths, (b) bond angles, and (c) dihedral angles.


(a)
B97D-B3LYP
wB97XD-B3LYP
CAM-B3LYP-B3LYP
0.012
0.008
0.004
0.000
-0.004
-0.008
-0.012
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D-B3LYP
wB97XD-B3LYP
CAM-B3LYP-B3LYP
0.4
0.2
0
-0.2
-0.4
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

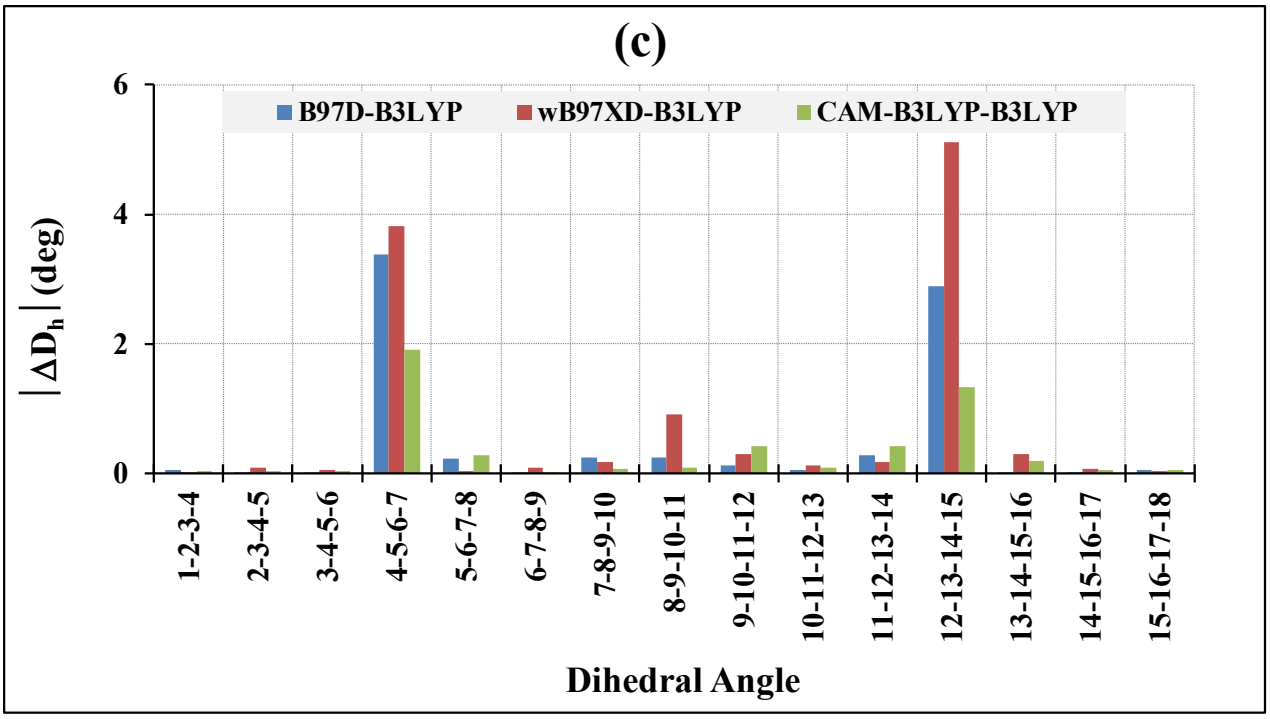
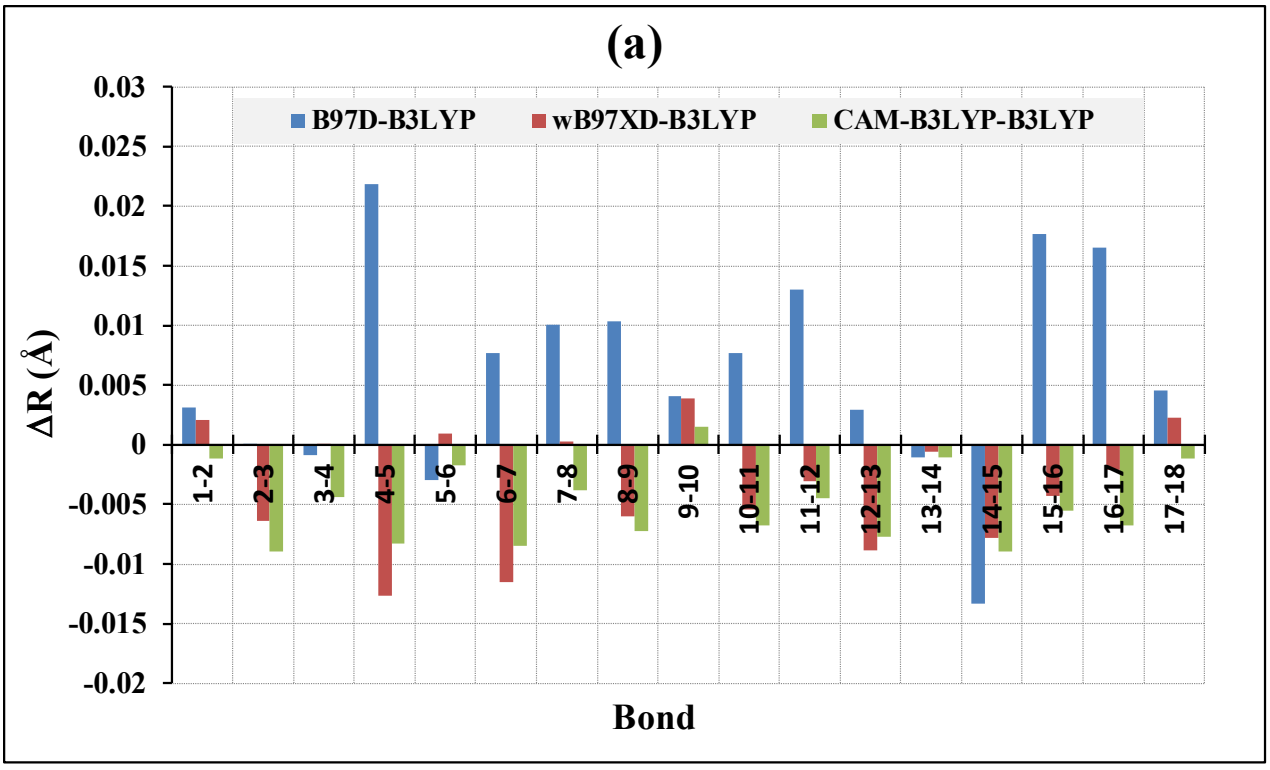
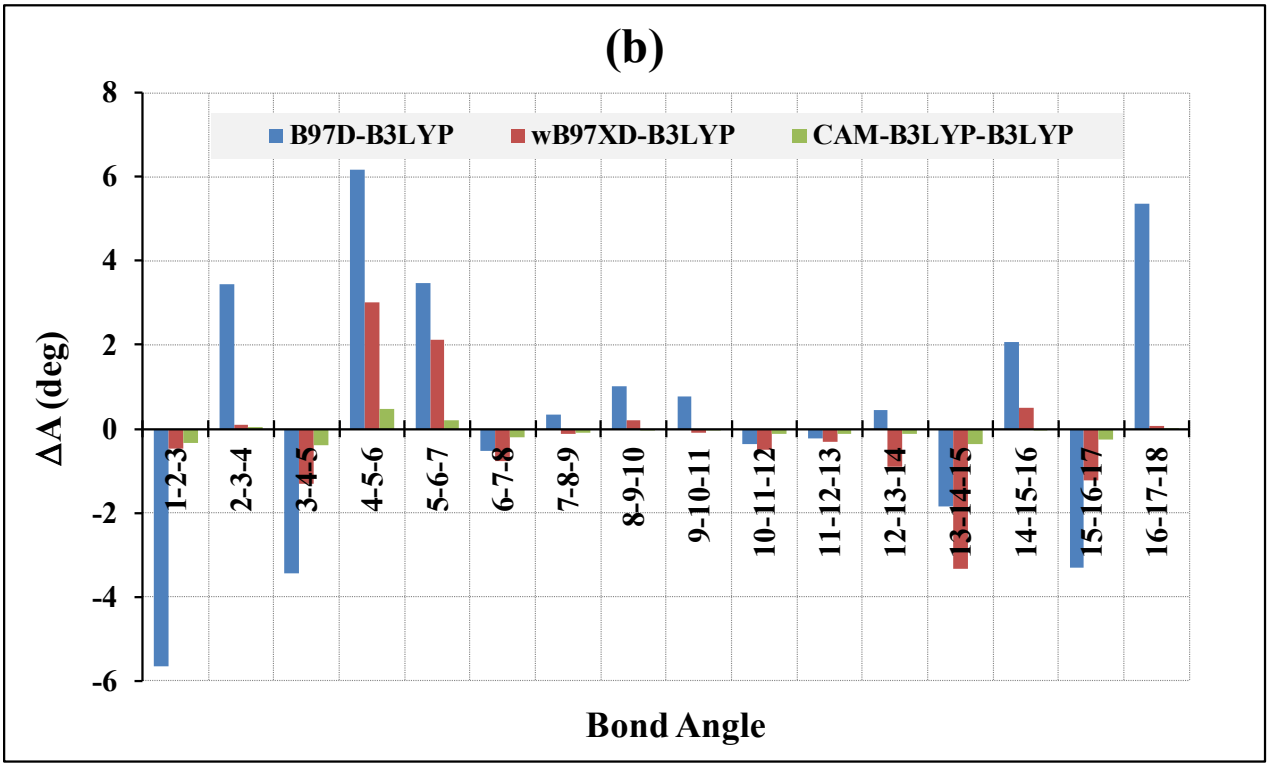


Figure S2. DFT method effect; comparison of the B3LYP geometrical parameters with other DFT methods' results for the isolated DPF-ALD with 2 SCs. The labeling of atoms is shown in Figure 1. This figure shows differences between (a) bond lengths, (b) bond angles, and (c) dihedral angles.


(a)
B97D-B3LYP
wB97XD-B3LYP
CAM-B3LYP-B3LYP
ΔR (Å)
0.03
0.025
0.02
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
-0.02
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D-B3LYP
wB97XD-B3LYP
CAM-B3LYP-B3LYP
ΔA (deg)
8
6
4
2
0
-2
-4
-6
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

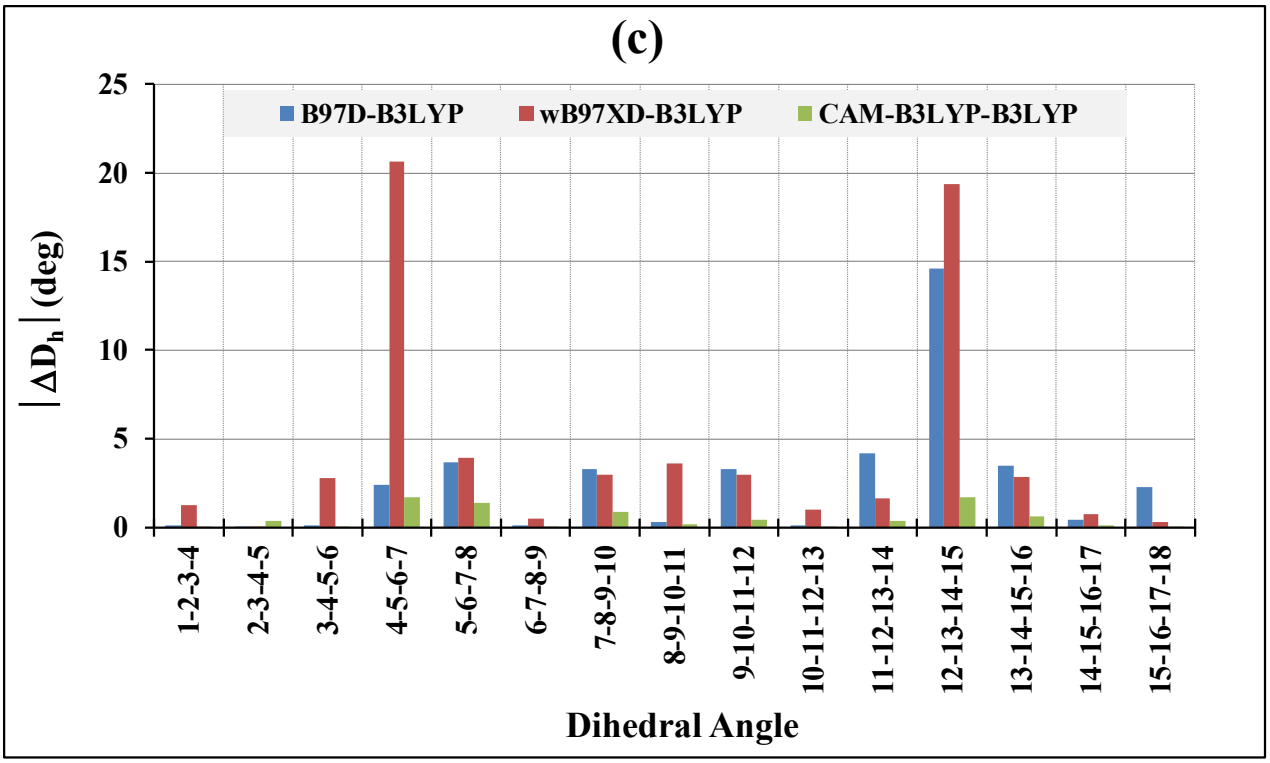
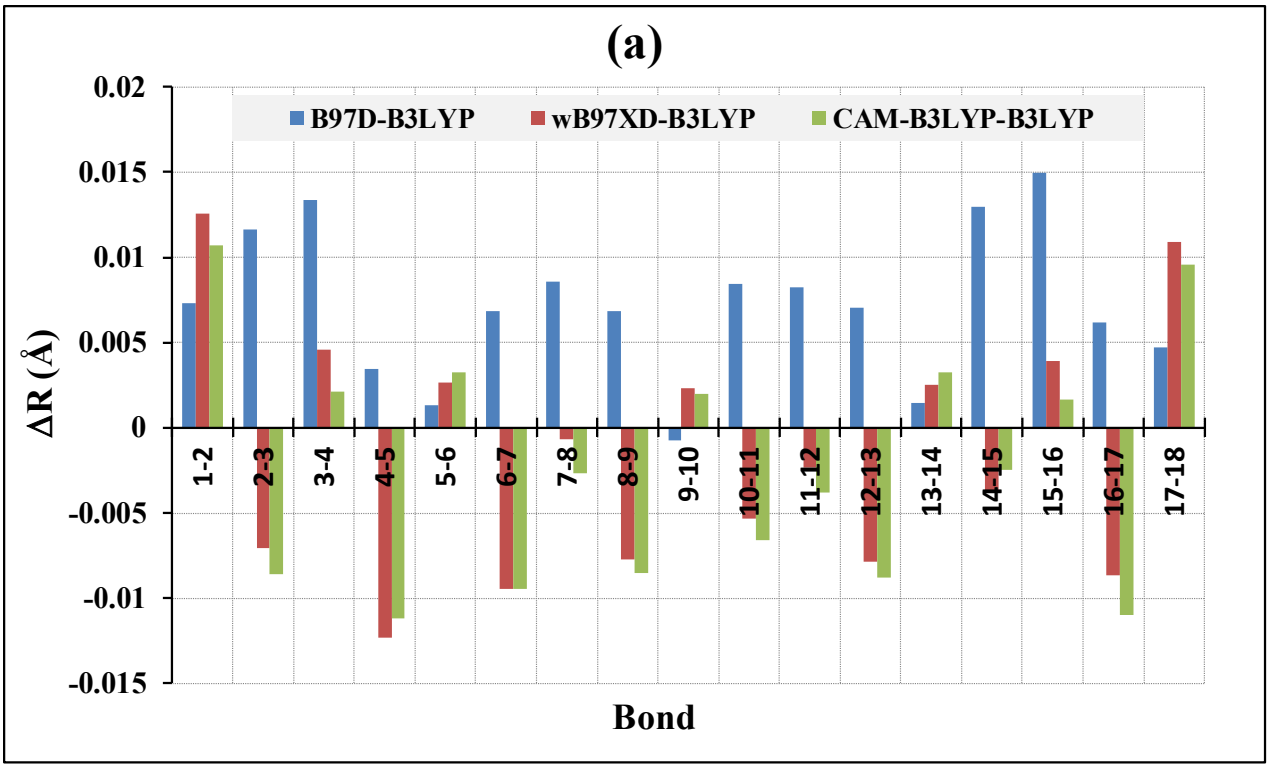
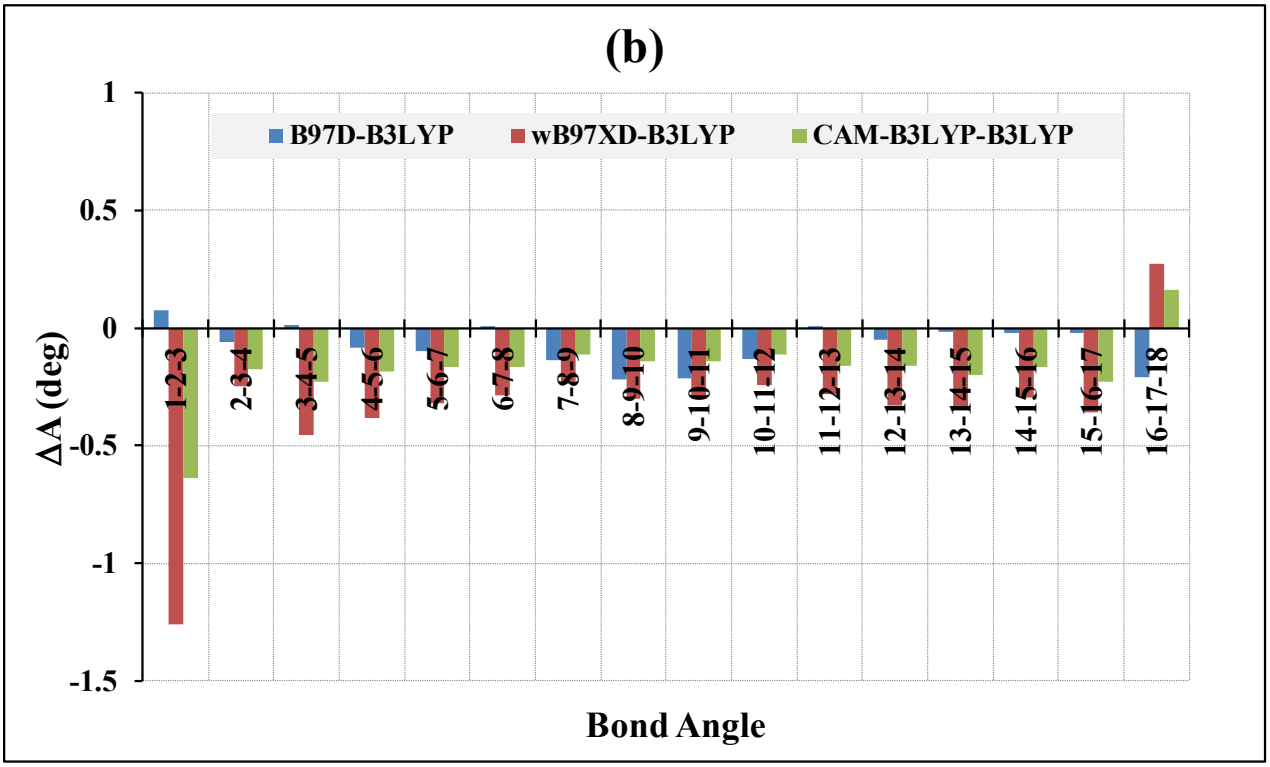


Figure S3. DFT method effect; comparison of the B3LYP geometrical parameters with other DFT methods' results for the isolated DPF-ALD with 6 SCs. The labeling of atoms is shown in Figure 1. This figure shows differences between (a) bond lengths, (b) bond angles, and (c) dihedral angles.


(a)
B97D-B3LYP
wB97XD-B3LYP
CAM-B3LYP-B3LYP
ΔR (Å)
0.02
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D-B3LYP
wB97XD-B3LYP
CAM-B3LYP-B3LYP
ΔA (deg)
1
0.5
0
-0.5
-1
-1.5
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

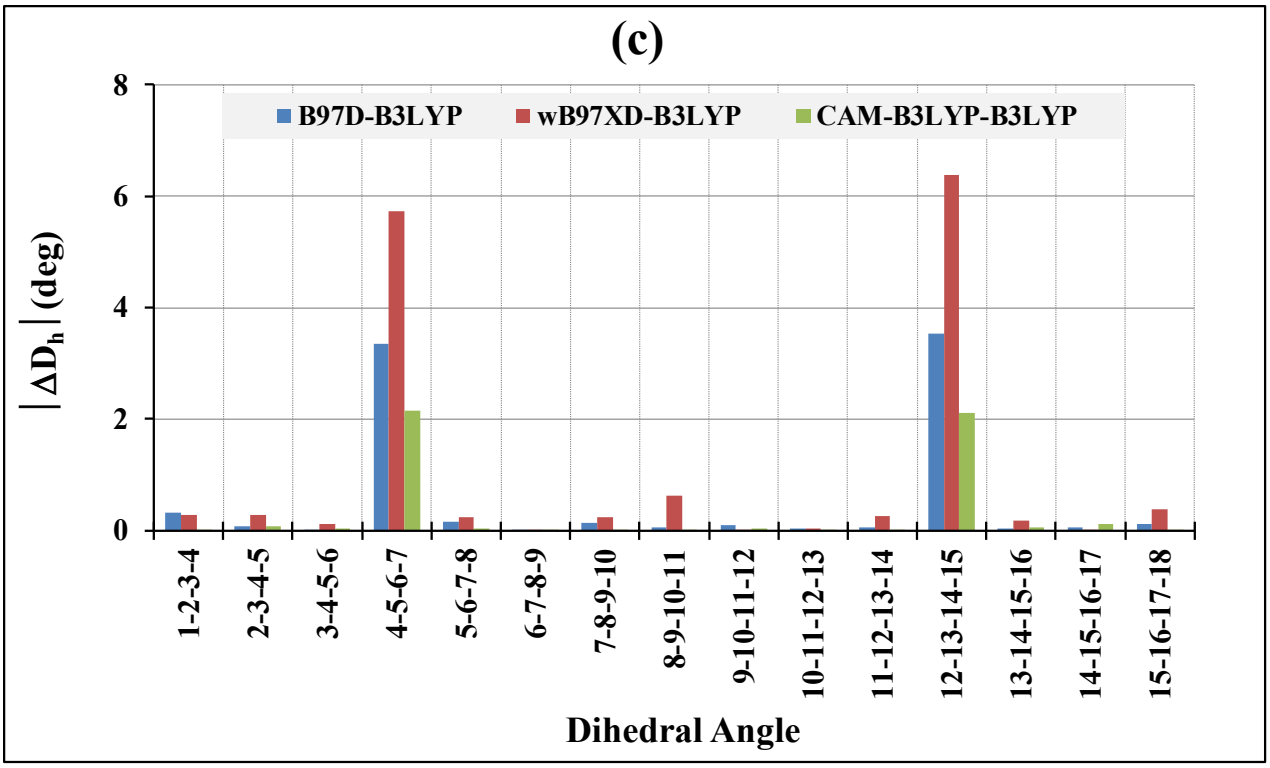
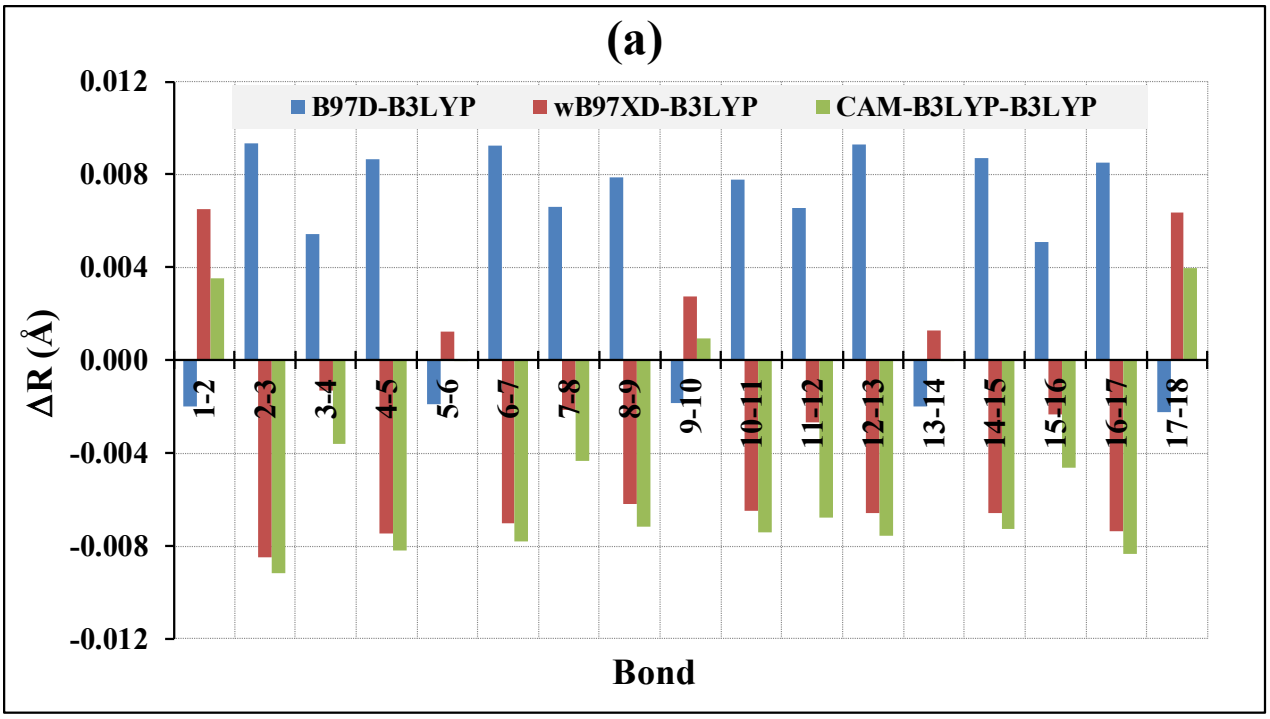
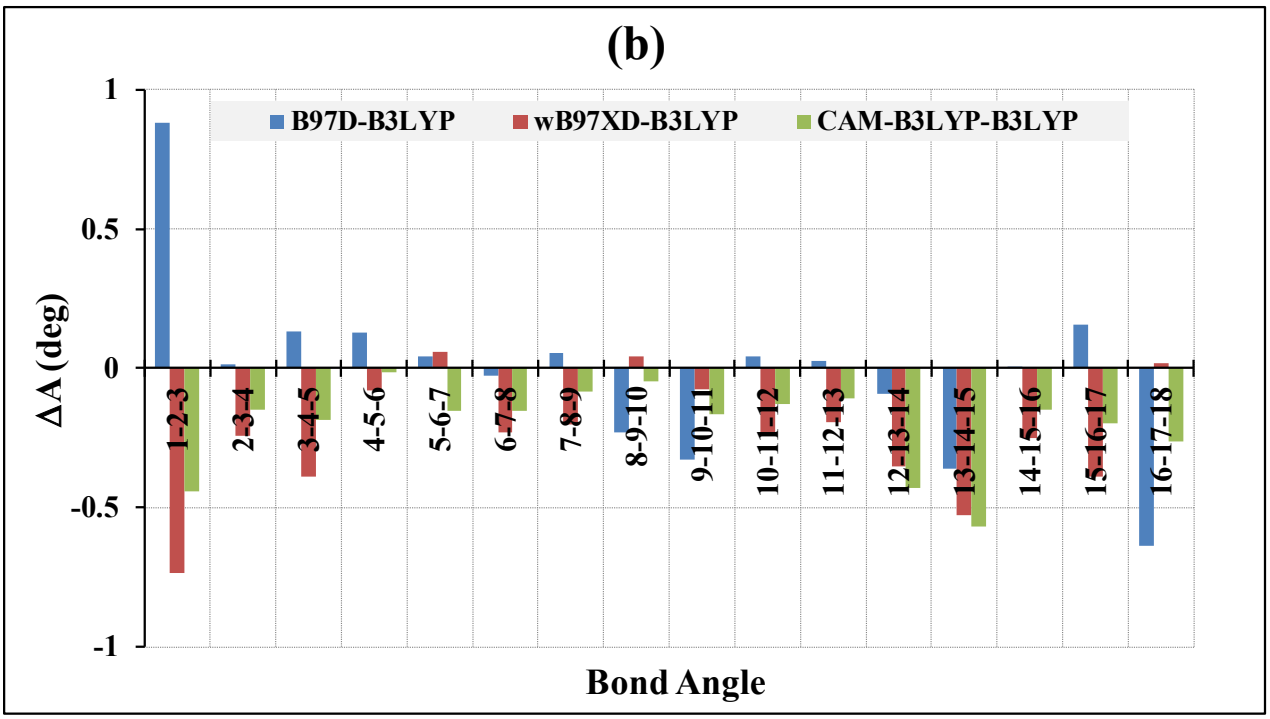


Figure S4. DFT method effect; comparison of the B3LYP geometrical parameters with other DFT methods' results for the isolated DPF-DTF without SCs. The labeling of atoms is shown in Figure 1. This figure shows differences between (a) bond lengths, (b) bond angles, and (c) dihedral angles.


(a)
B97D-B3LYP
wB97XD-B3LYP
CAM-B3LYP-B3LYP
0.012
0.008
0.004
0.000
-0.004
-0.008
-0.012
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D-B3LYP
wB97XD-B3LYP
CAM-B3LYP-B3LYP
1
0.5
0
-0.5
-1
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

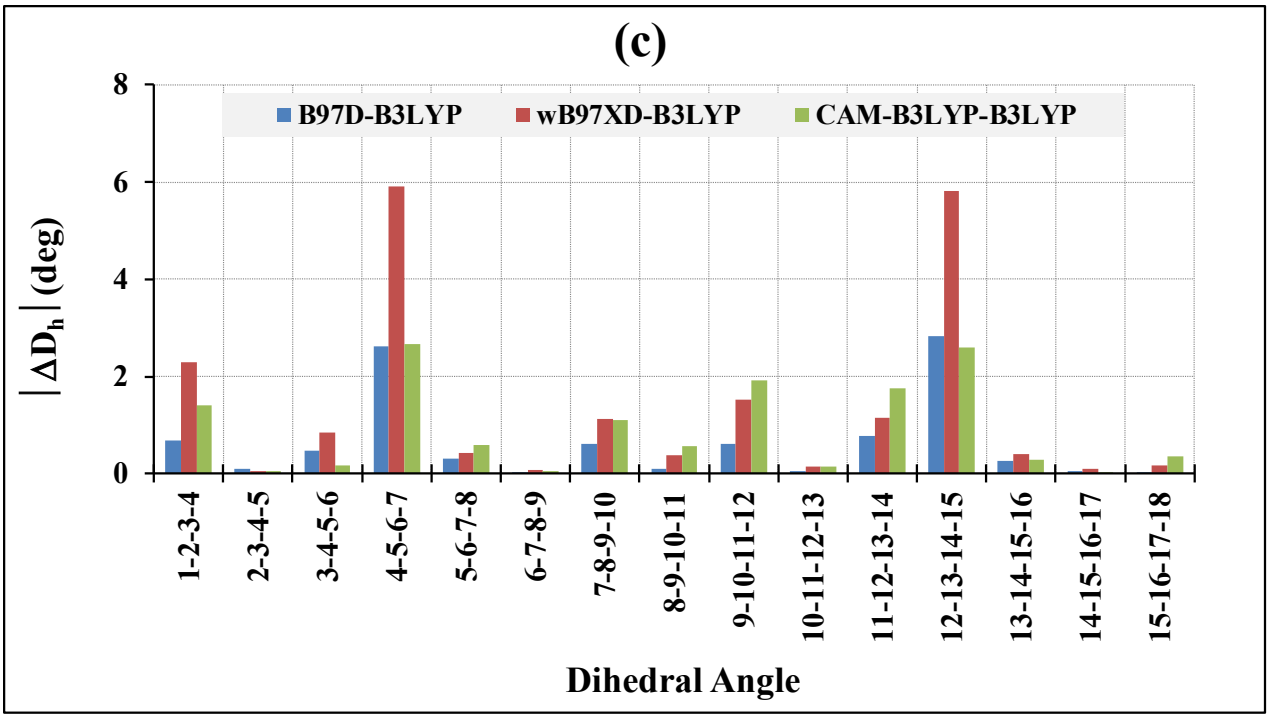
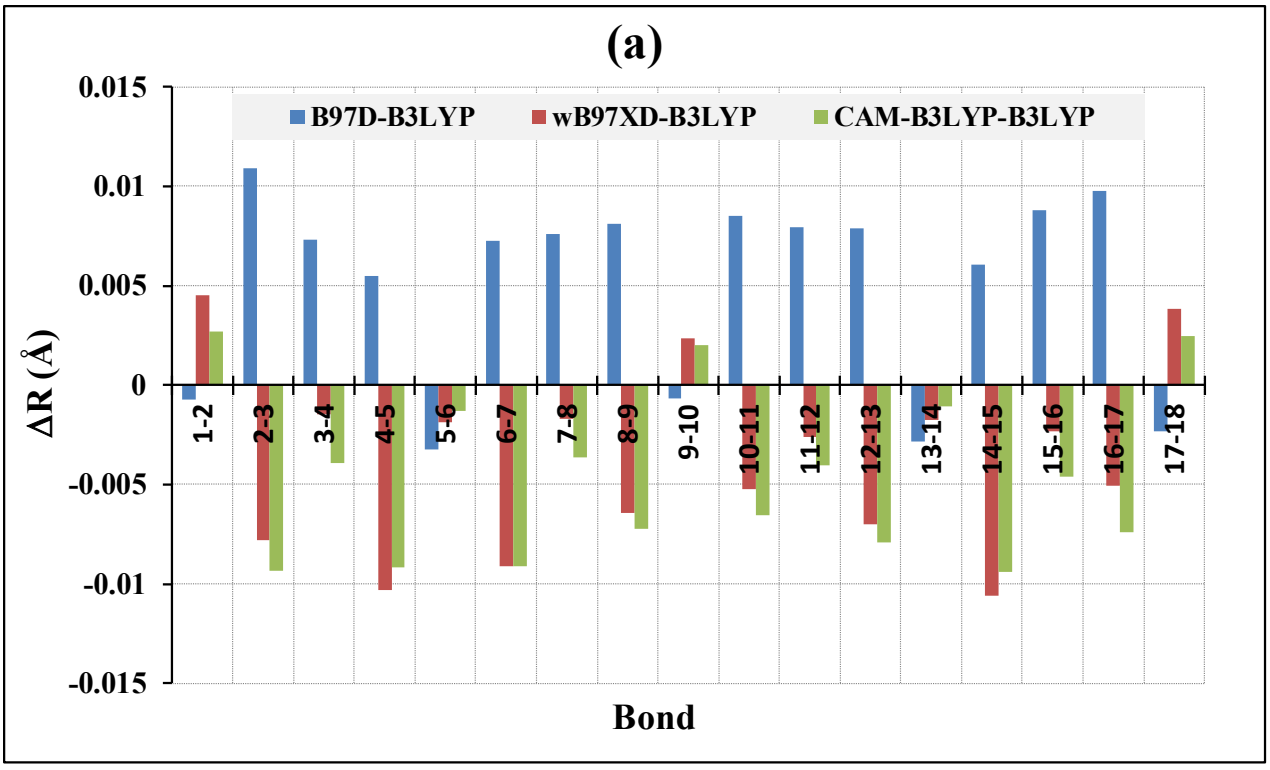
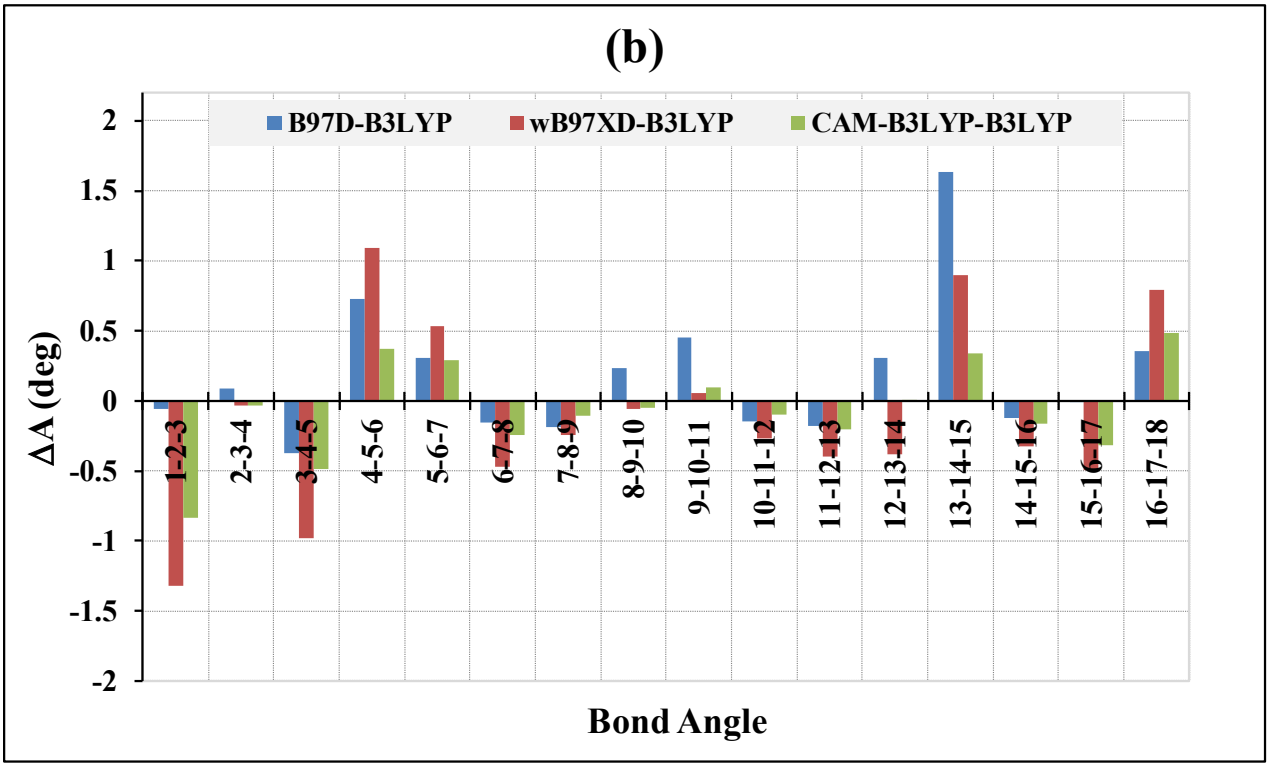


Figure S5. DFT method effect; comparison of the B3LYP geometrical parameters with other DFT methods' results for the isolated DPF-DTF with 6 SCs. The labeling of atoms is shown in Figure 1. This figure shows differences between (a) bond lengths, (b) bond angles, and (c) dihedral angles.


(a)
B97D-B3LYP
wB97XD-B3LYP
CAM-B3LYP-B3LYP
ΔR (Å)
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D-B3LYP
wB97XD-B3LYP
CAM-B3LYP-B3LYP
ΔA (deg)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

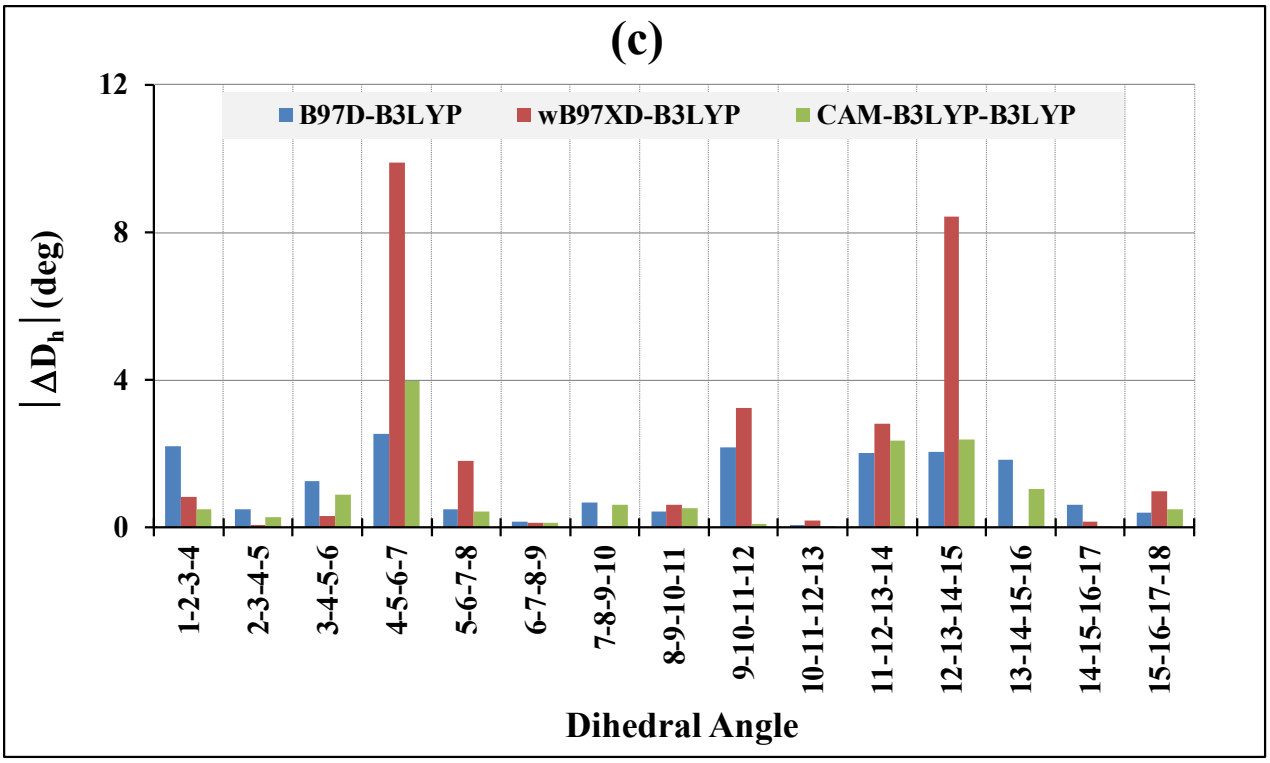
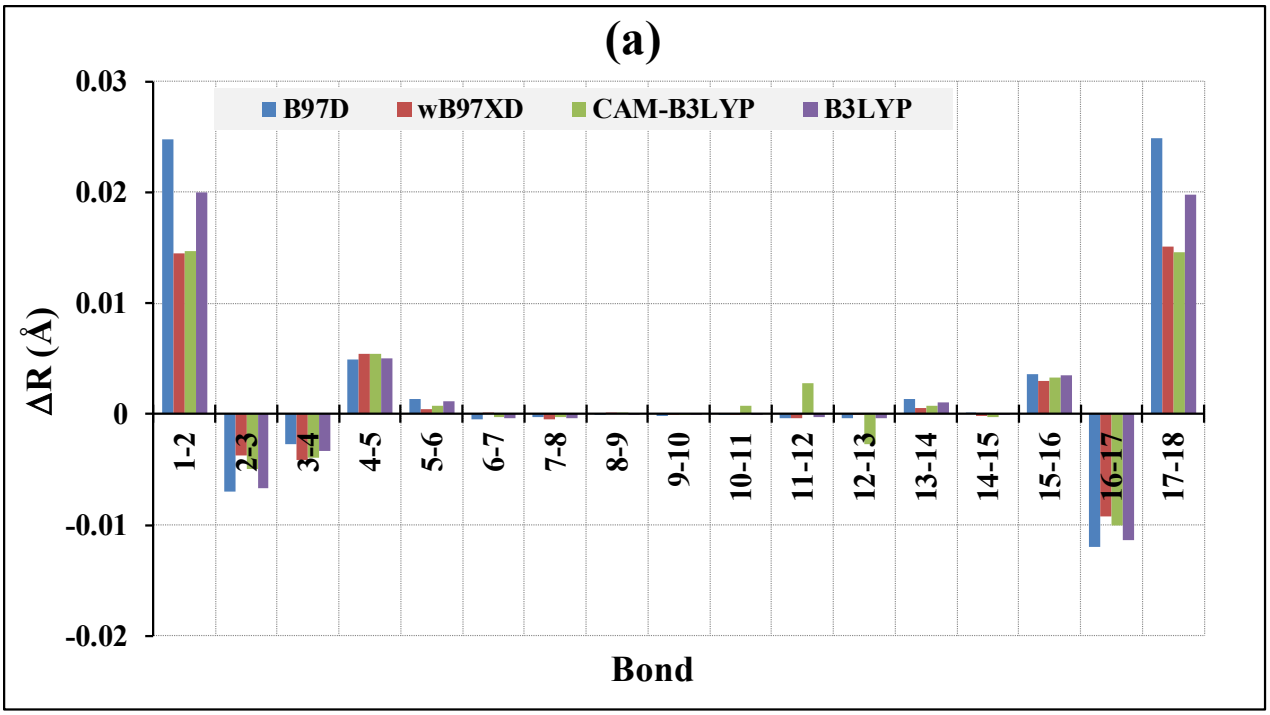
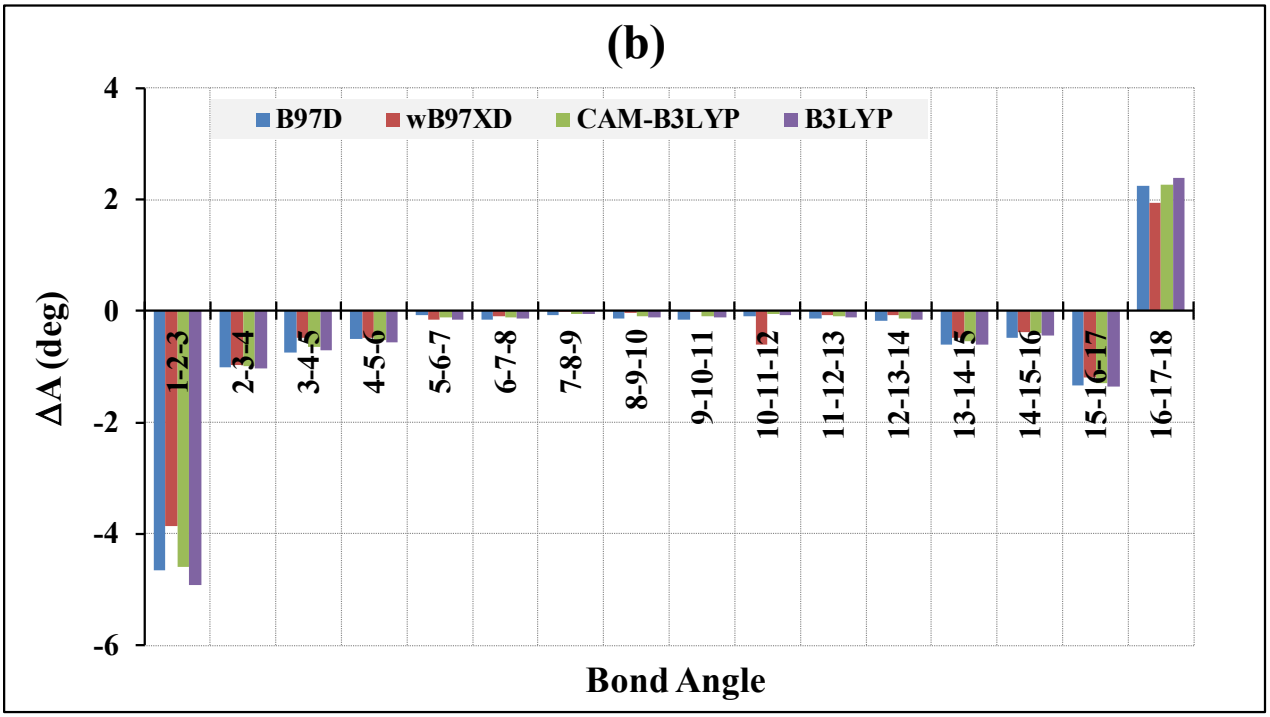


Figure S6. DFT method effect; comparison of the B3LYP geometrical parameters with other DFT methods' results for the isolated DPF-DTF with 10 SCs. The labeling of atoms is shown in Figure 1. This figure shows differences between (a) bond lengths, (b) bond angles, and (c) dihedral angles.


(a)
B97D
wB97XD
CAM-B3LYP
B3LYP
0.03
0.02
0.01
0
-0.01
-0.02
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
B3LYP
4
2
0
-2
-4
-6
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

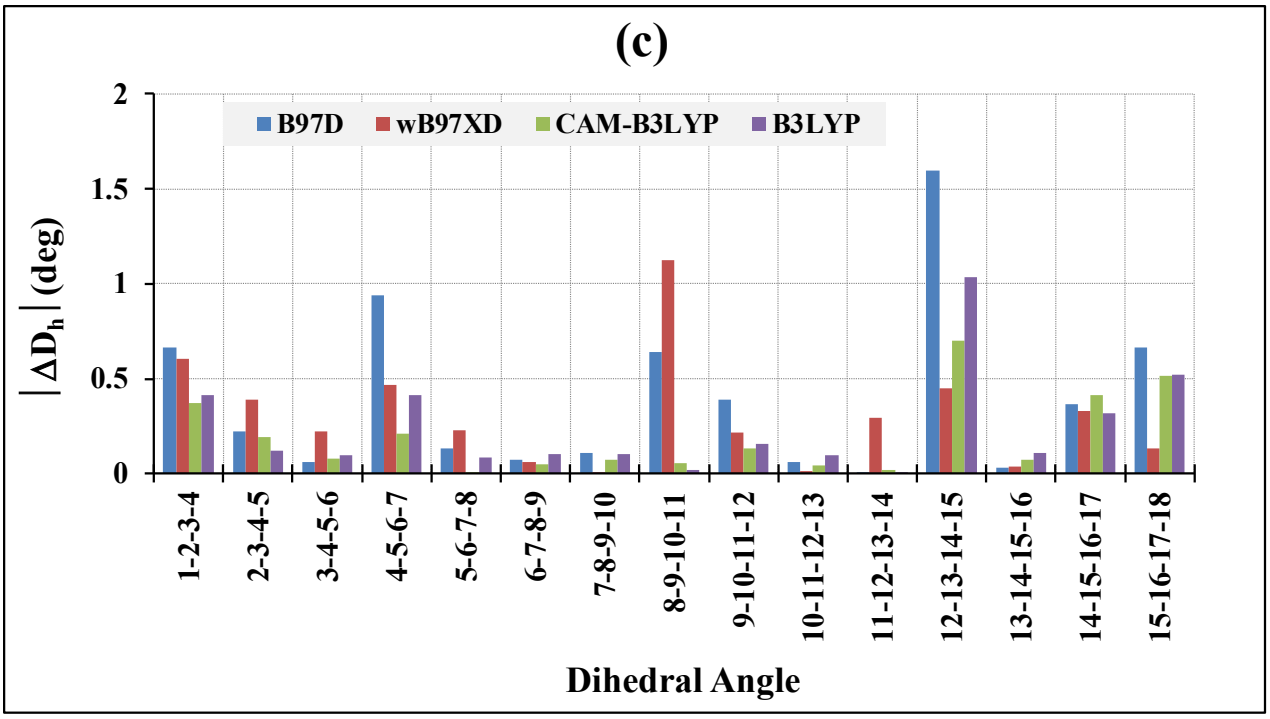
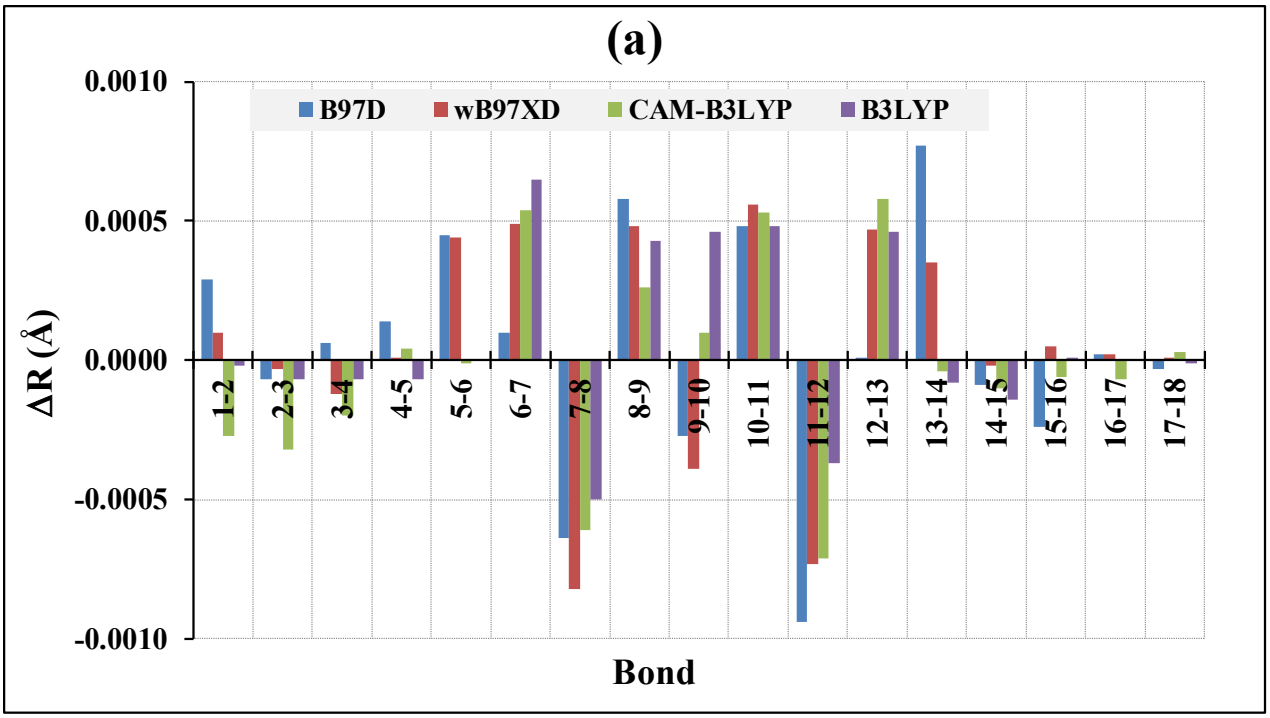
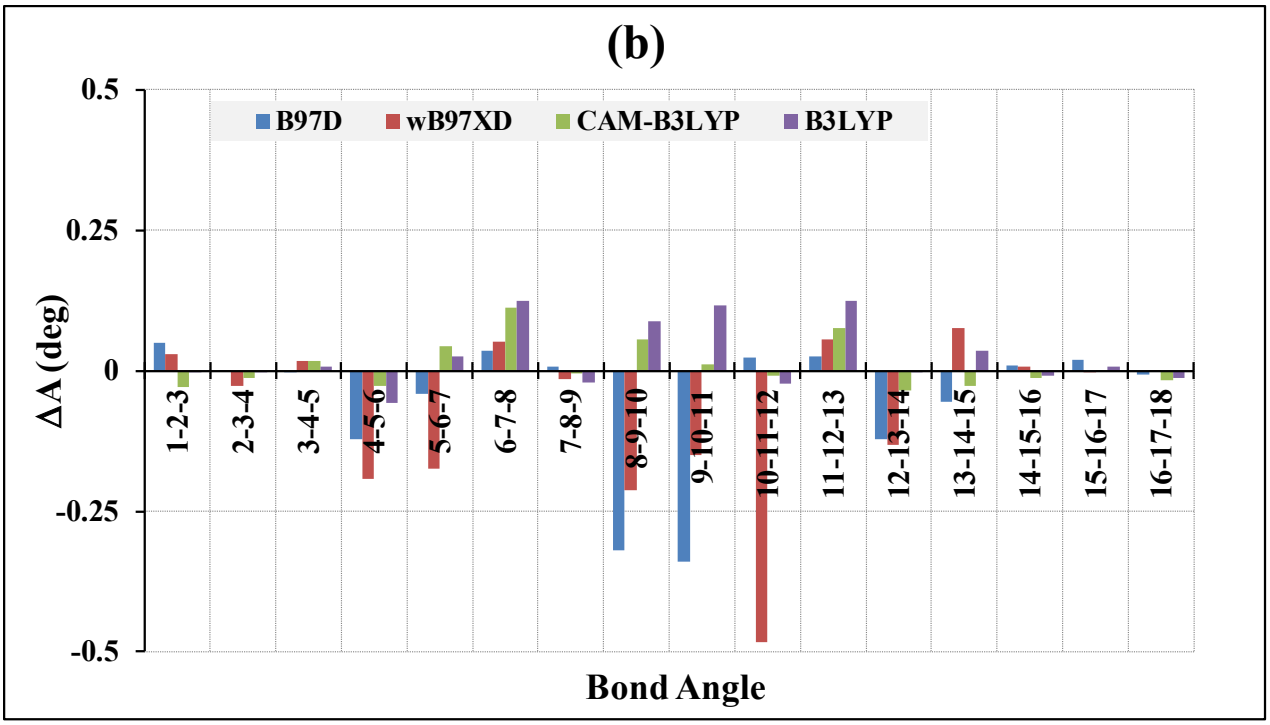


Figure S7. End group effect; differences between the geometrical parameters of the isolated DPF-ALD and DPF-DTF (without SCs) obtained using four DFT methods (as indicated in the figure) with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1. This figure shows the differences between (a) bond lengths, (b) bond angles and (c) dihedral angles.


(a)
B97D
wB97XD
CAM-B3LYP
B3LYP
0.0010
0.0005
0.0000
-0.0005
-0.0010
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
B3LYP
0.5
0.25
0
-0.25
-0.5
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

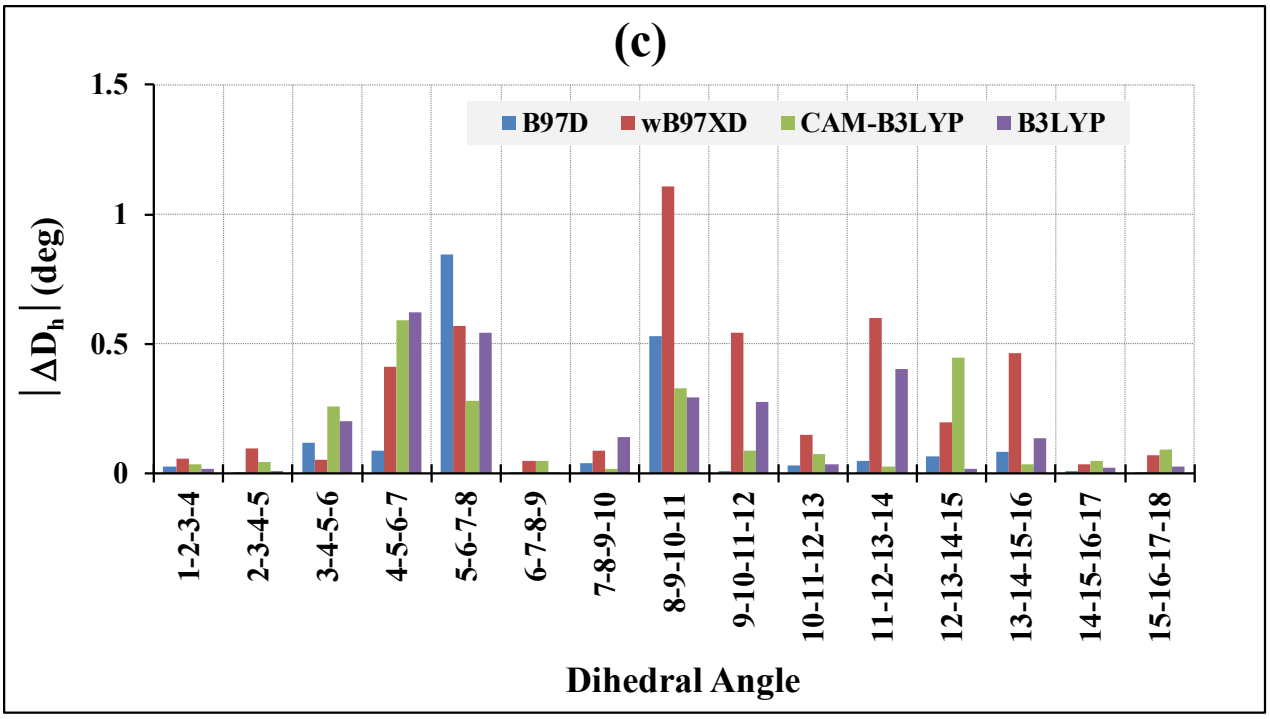
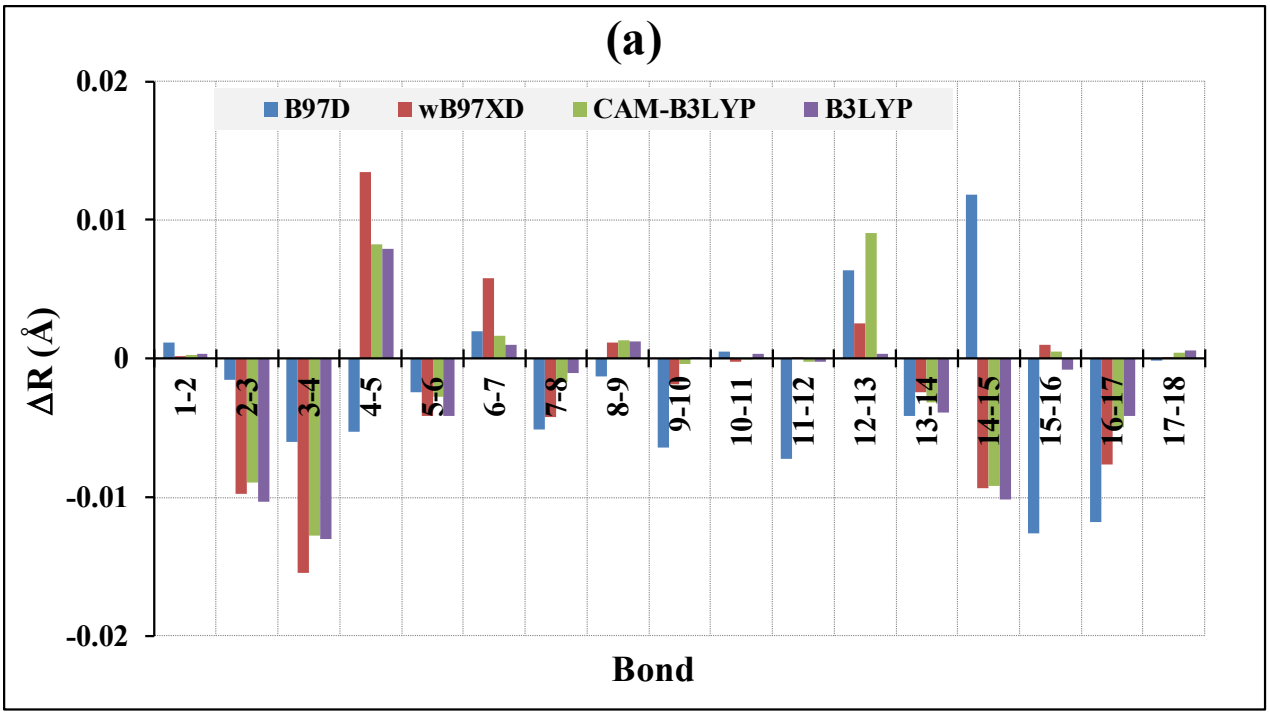
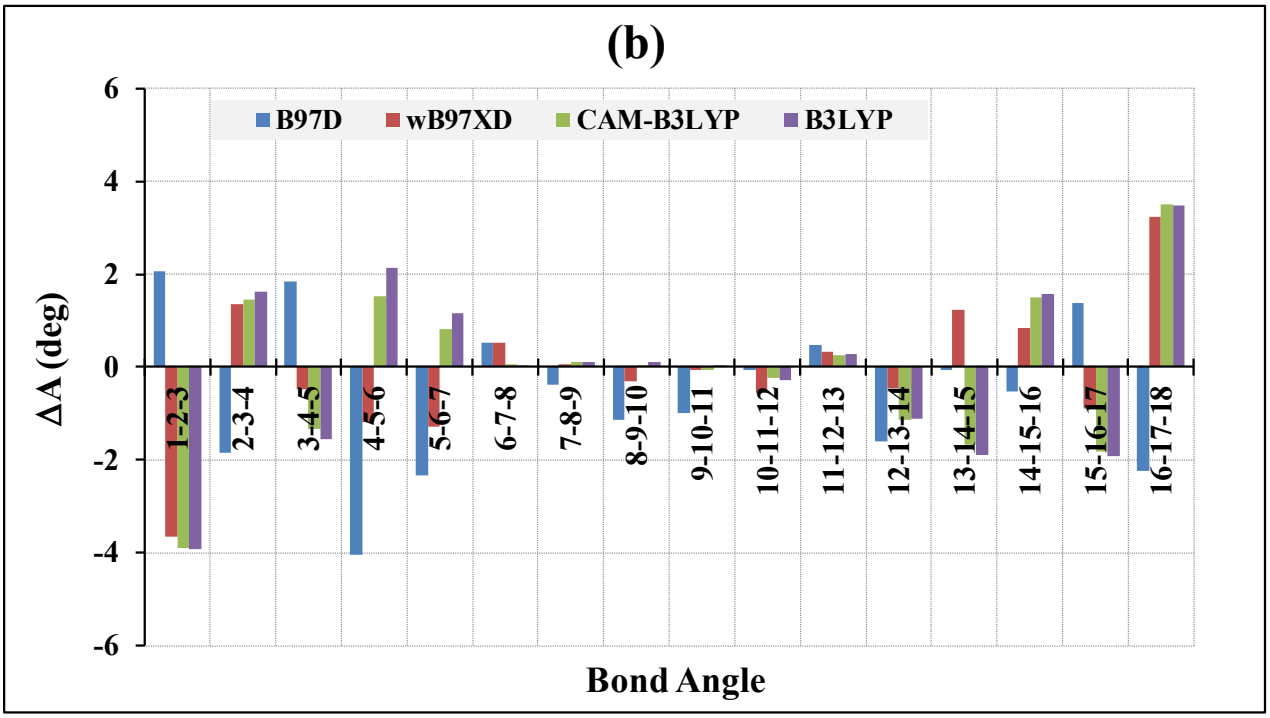


Figure S8. Side chain effect; differences between the geometrical parameters of the isolated DPF-ALD with 2 SCs and DPF-ALD without SCs obtained using four DFT methods (as indicated in the figure) with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1. This figure shows the differences between (a) bond lengths, (b) bond angles and (c) dihedral angles.


(a)
B97D
wB97XD
CAM-B3LYP
B3LYP
0.02
0.01
0
-0.01
-0.02
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
B3LYP
6
4
2
0
-2
-4
-6
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

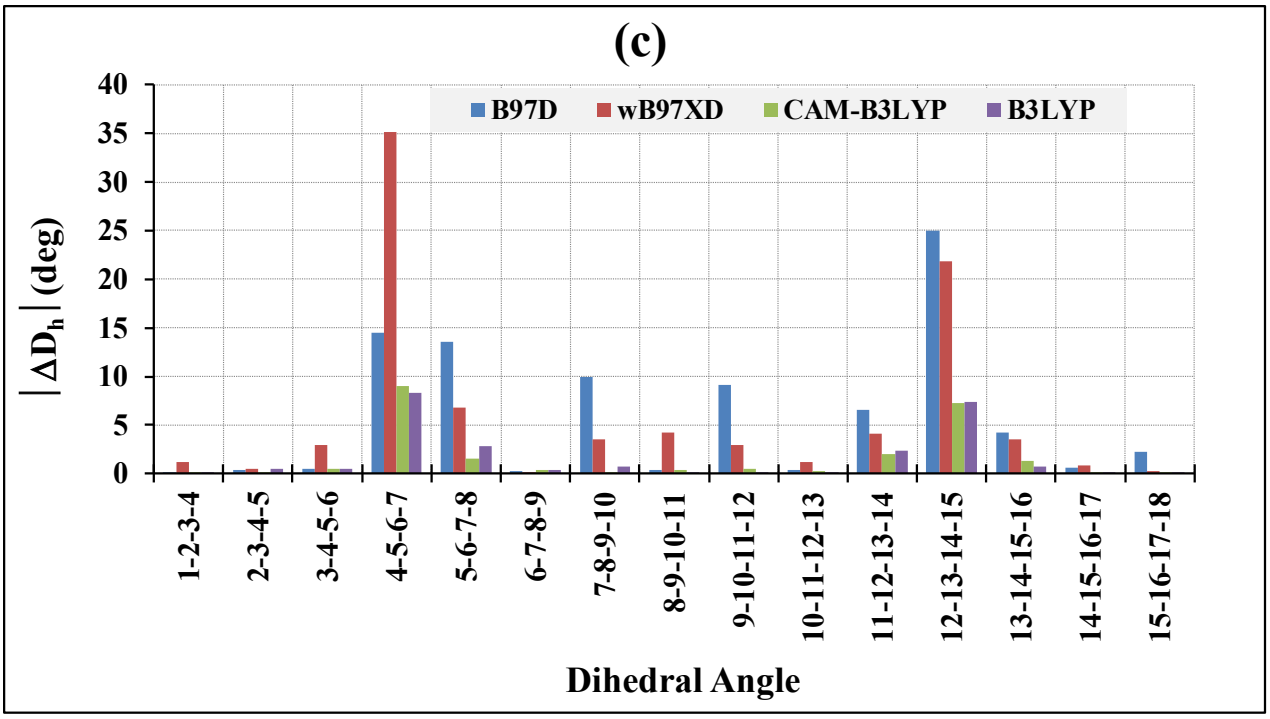
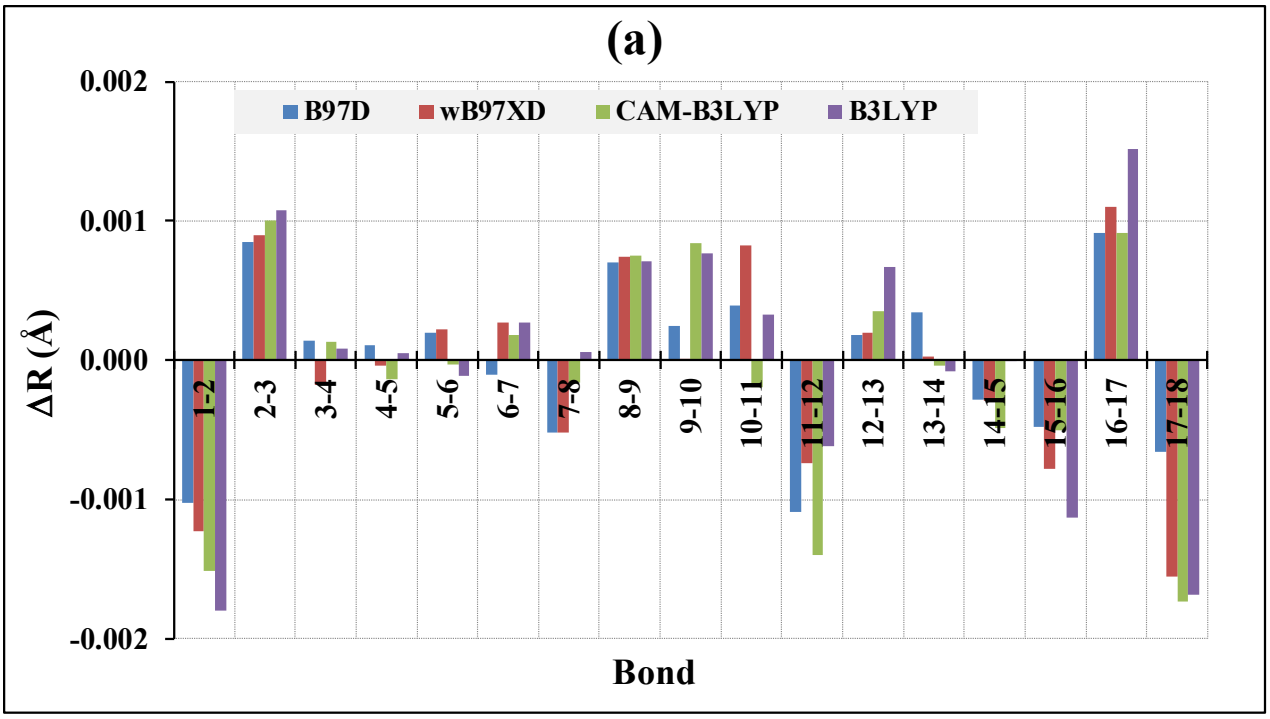
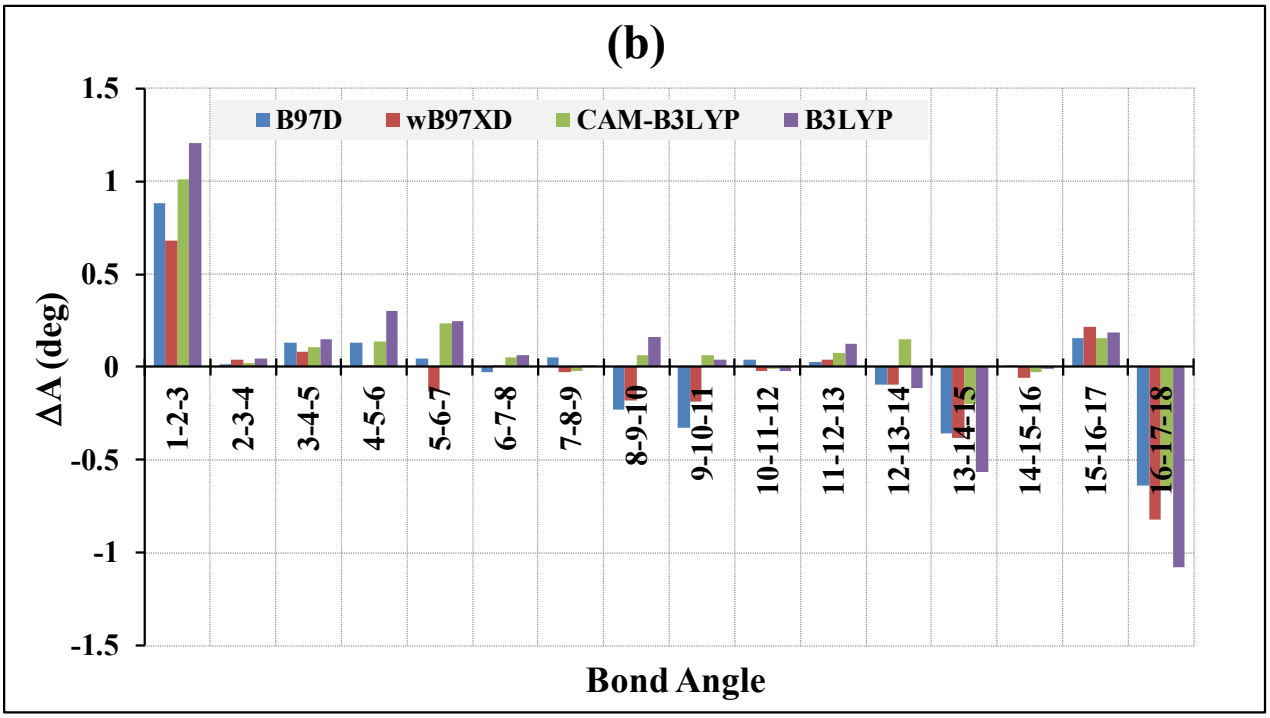


Figure S9. Side chain effect; differences between the geometrical parameters of the isolated DPF-ALD with 6 SCs and DPF-ALD without SCs obtained using four DFT methods (as indicated in the figure) with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1. This figure shows the differences between (a) bond lengths, (b) bond angles and (c) dihedral angles.


(a)
B97D
wB97XD
CAM-B3LYP
B3LYP
0.002
0.001
0.000
-0.001
-0.002
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
B3LYP
1.5
1
0.5
0
-0.5
-1
-1.5
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

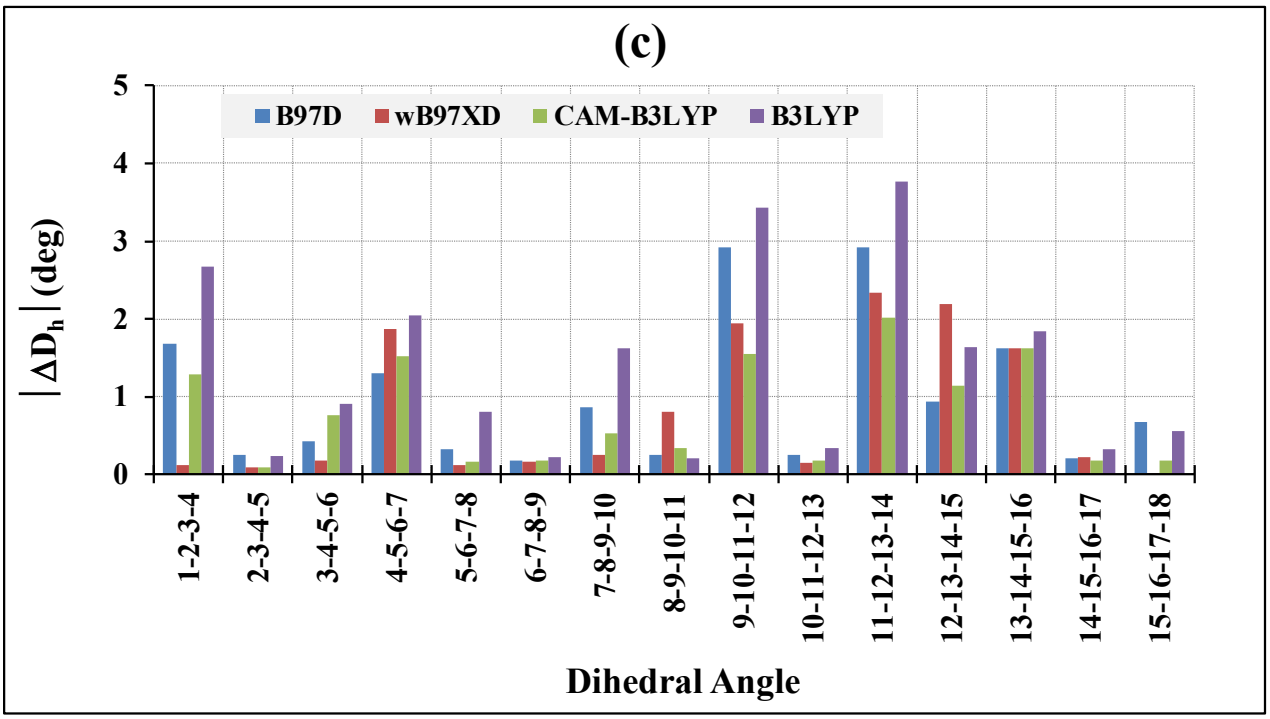
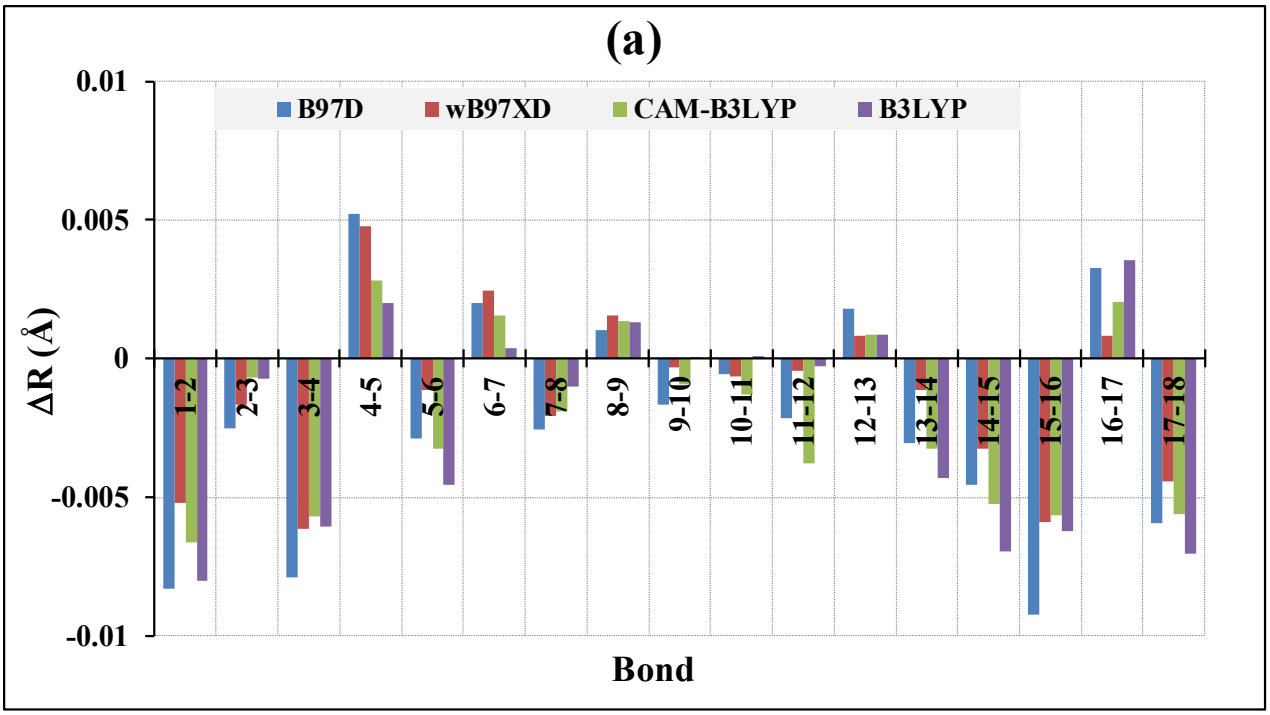
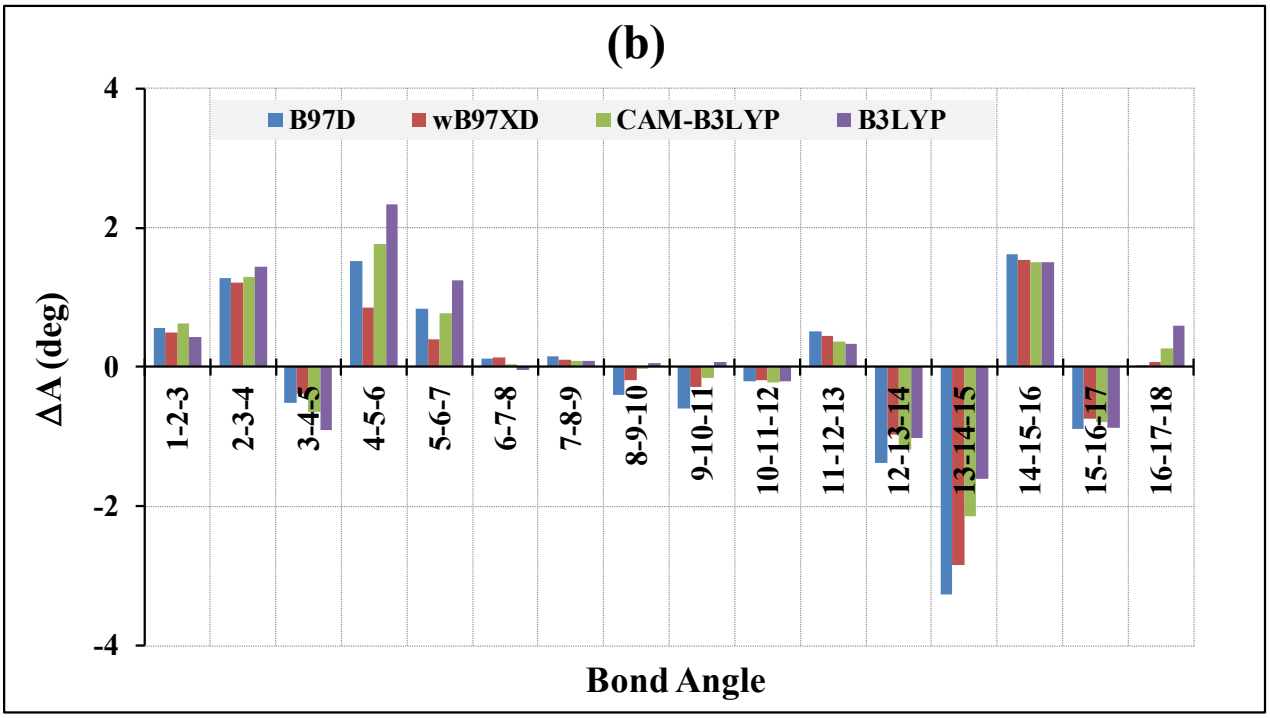


Figure S10. Side chain effect; differences between the geometrical parameters of the isolated DPF-DTF with 6 SCs and DPF-DTF without SCs obtained using four DFT methods (as indicated in the figure) with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1. This figure shows the differences between (a) bond lengths, (b) bond angles and (c) dihedral angles.


(a)
B97D
wB97XD
CAM-B3LYP
B3LYP
0.01
0.005
0
-0.005
-0.01
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
B3LYP
4
2
0
-2
-4
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

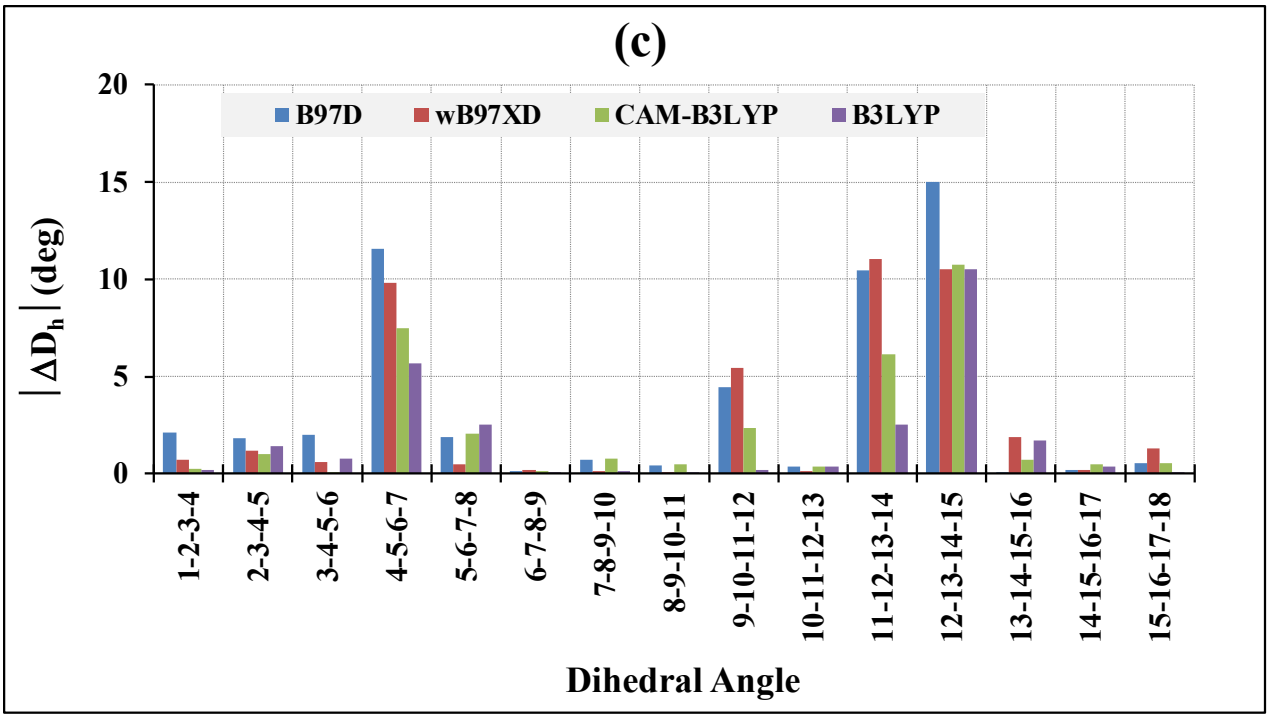


Figure S11. Side chain effect; differences between the geometrical parameters of the isolated DPF-DTF with 10 SCs and DPF-DTF without SCs obtained using four DFT methods (as indicated in the figure) with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1. This figure shows the differences between (a) bond lengths, (b) bond angles and (c) dihedral angles.

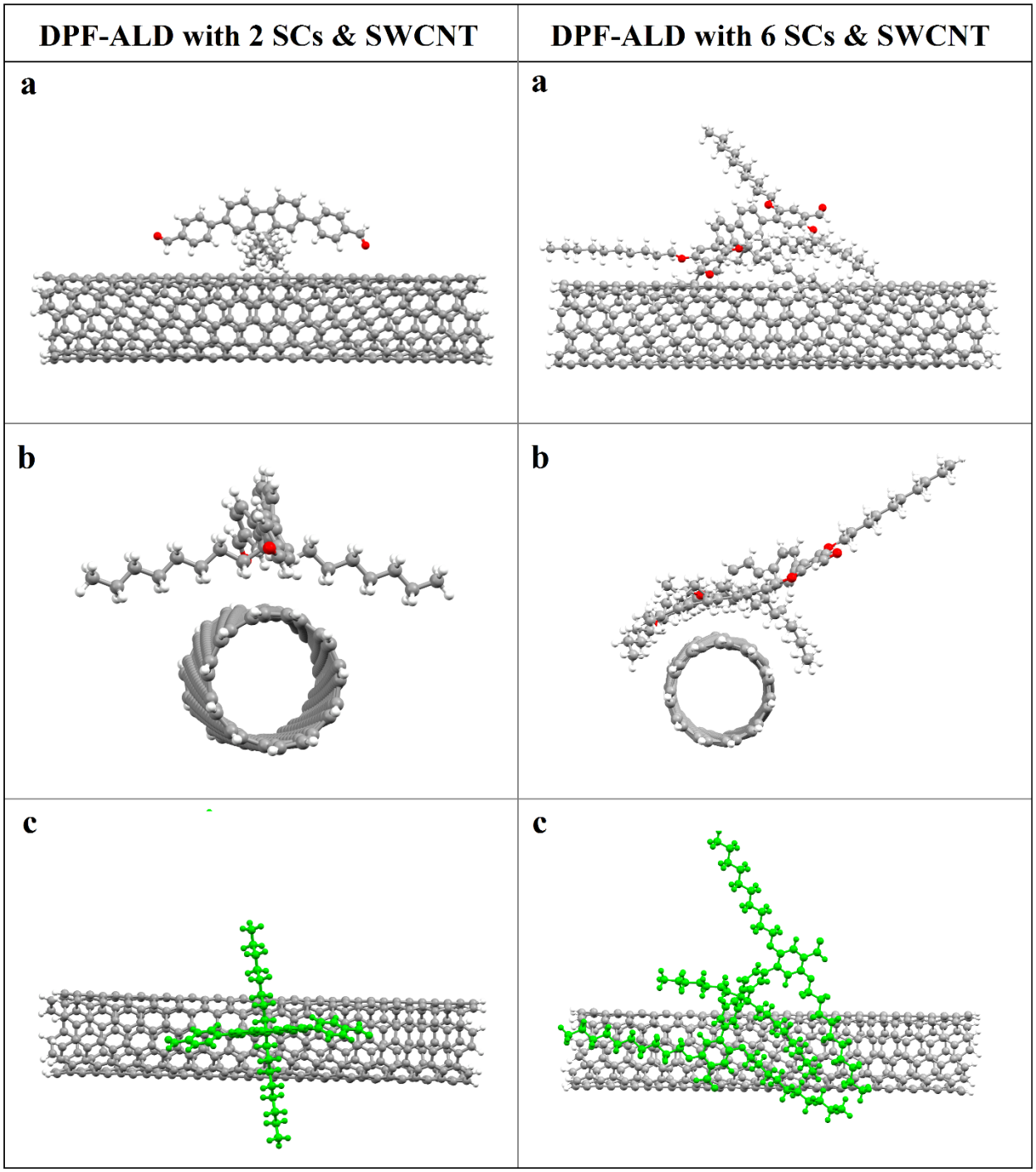


Figure S12. Representative (partially) optimized structures of DPF-ALD molecules with SCs interacting with the (6,5) SWCNT obtained using B97D with 6-31G(d) basis set; (a) side view, (b) front view, and (c) top view with the oligomers highlighted.

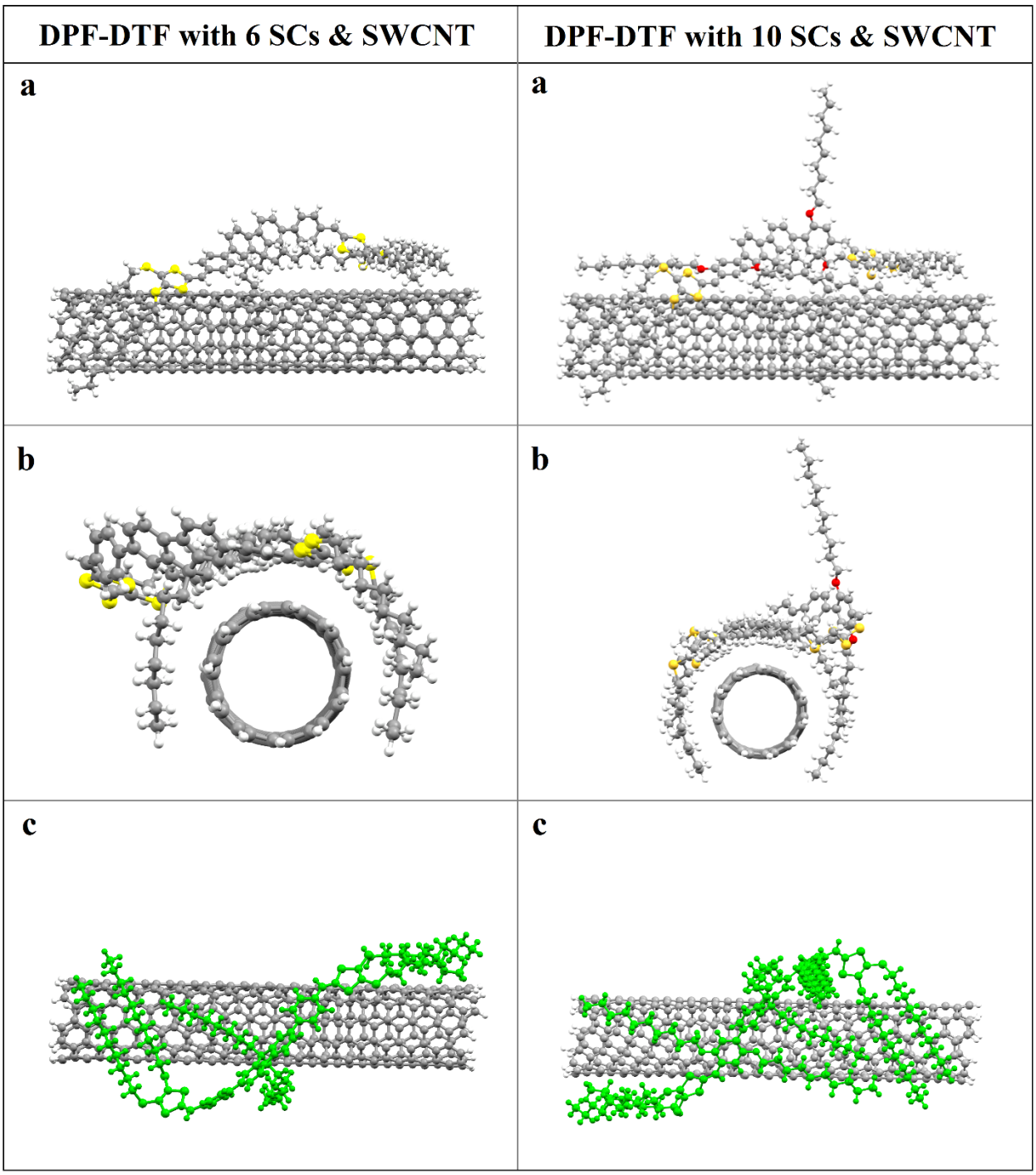


Figure S13. Representative (partially) optimized structures of DPF-DTF molecules with SCs interacting with the (6,5) SWCNT obtained using B97D with 6-31G(d) basis set; (a) side view, (b) front view, and (c) top view with the oligomers highlighted.

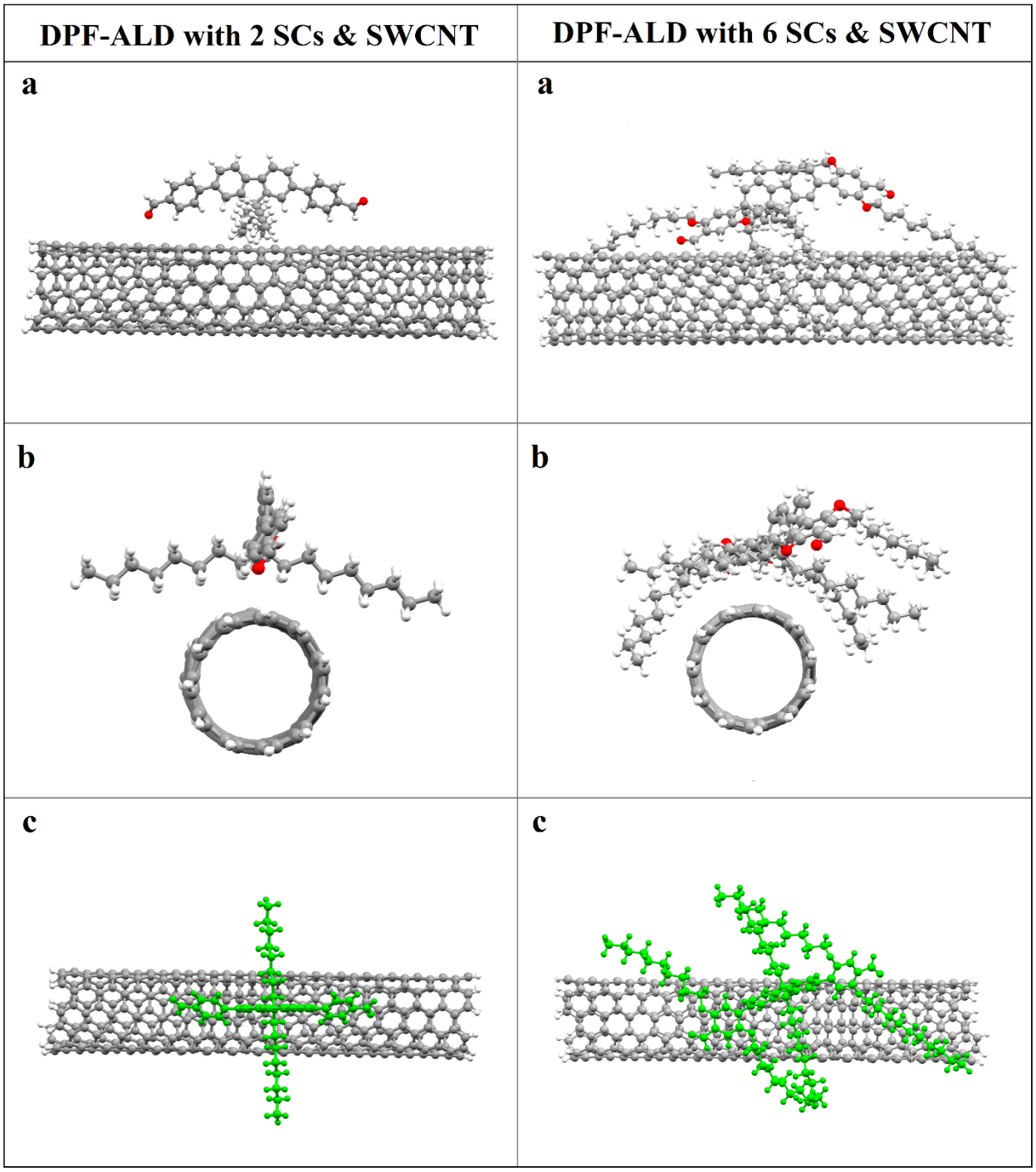


Figure S14. Representative (partially) optimized structures of DPF-ALD molecules with SCs interacting with the (6,5) SWCNT obtained using wB97XD with 6-31G(d) basis set; (a) side view, (b) front view, and (c) top view with the oligomers highlighted.

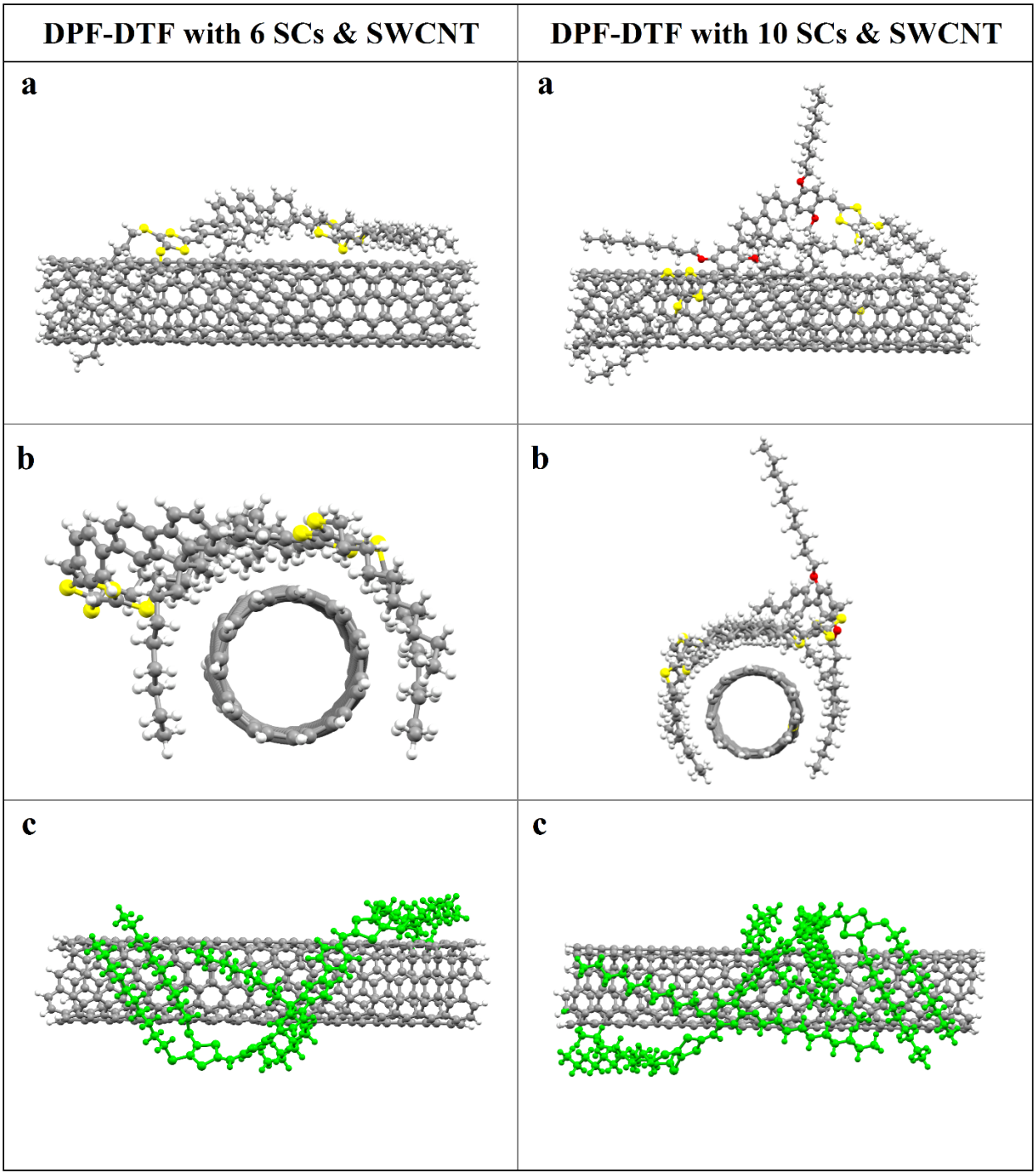


Figure S15. Representative (partially) optimized structures of DPF-DTF molecules with SCs interacting with the (6,5) SWCNT obtained using wB97XD with 6-31G(d) basis set; (a) side view, (b) front view, and (c) top view with the oligomers highlighted.

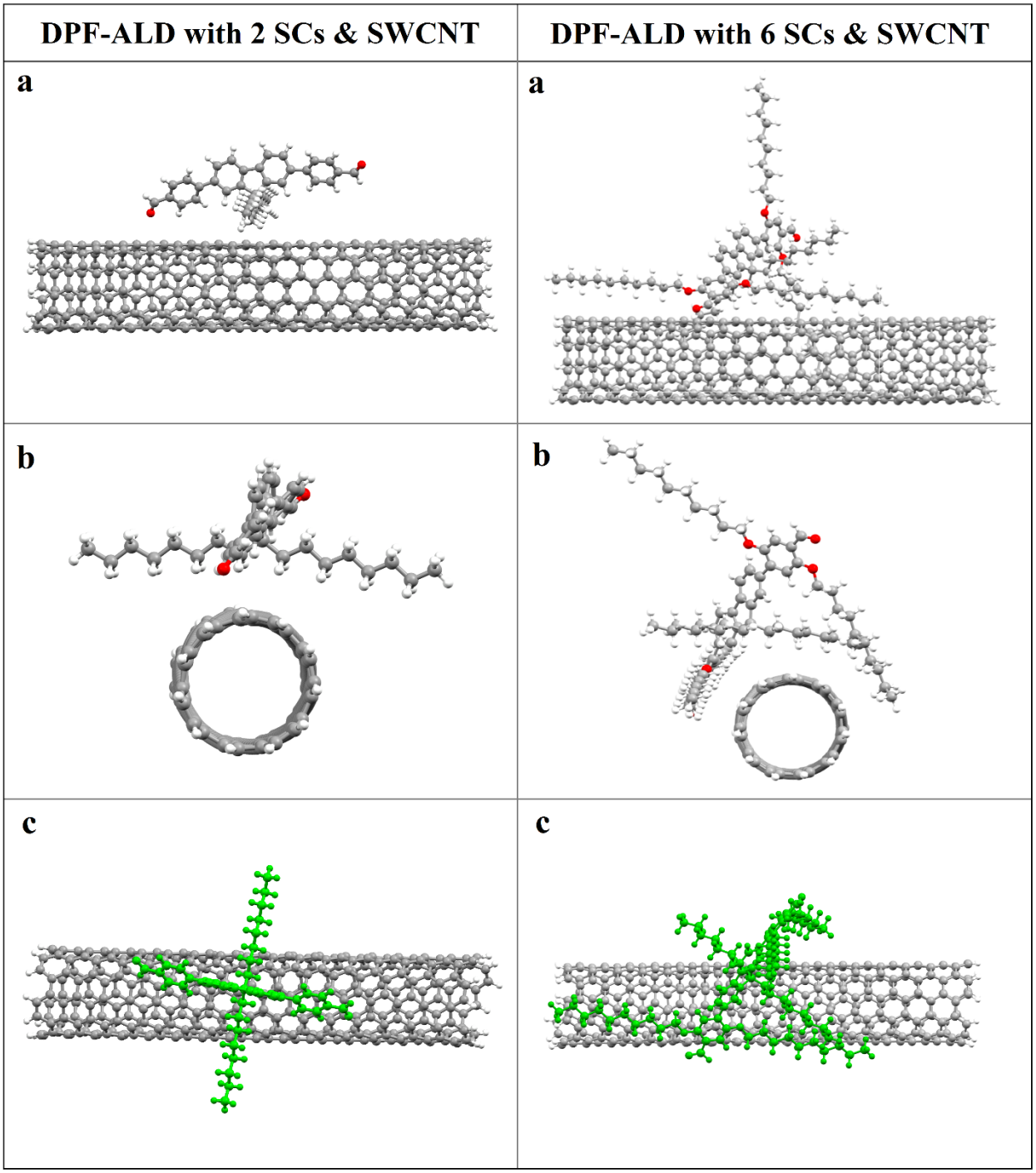


Figure S16. Representative (partially) optimized structures of DPF-ALD molecules with SCs interacting with the (6,5) SWCNT obtained using CAM-B3LYP with 6-31G(d) basis set; (a) side view, (b) front view, and (c) top view with the oligomers highlighted.

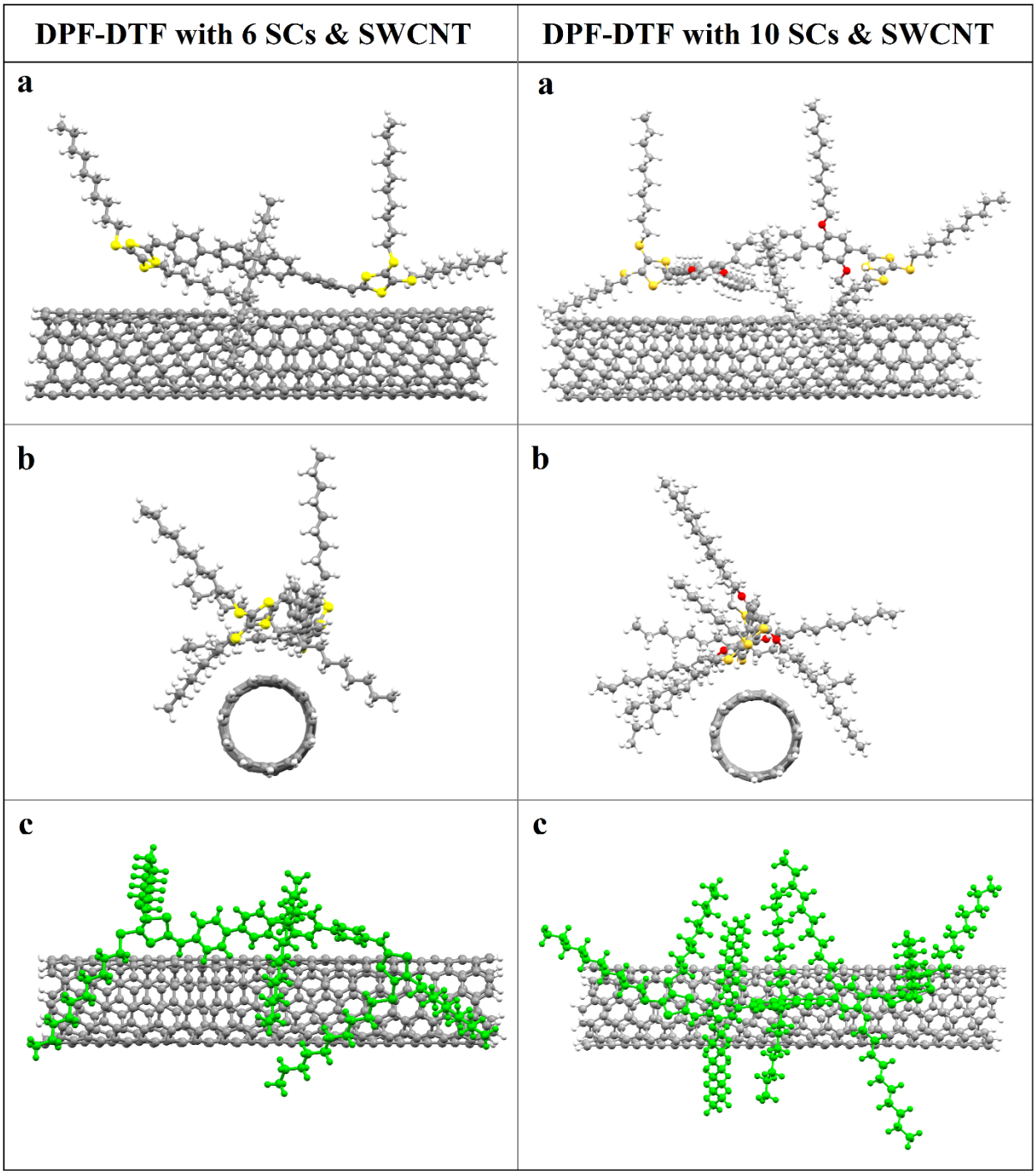


Figure S17. Representative (partially) optimized structures of DPF-DTF molecules with SCs interacting with the (6,5) SWCNT obtained using CAM-B3LYP with 6-31G(d) basis set; (a) side view, (b) front view, and (c) top view with the oligomers highlighted.

Table S7. Selected bond lengths (R) (in Å), bond angles (A) (in degrees), and dihedral angles (D_h) (in degrees) of DPF-ALD without SCs interacting with (6,5) SWCNT. The labeling of atoms is shown in Figure 1.

Bond Length (R)	**B97D**	**wB97XD**	**CAM-B3LYP**
R_{1-2}	1.478	1.478	1.476
R_{2-3}	1.411	1.397	1.396
R_{3-4}	1.392	1.383	1.383
R_{4-5}	1.421	1.406	1.403
R_{5-6}	1.483	1.486	1.482
R_{6-7}	1.419	1.404	1.402
R_{7-8}	1.397	1.389	1.388
R_{8-9}	1.403	1.390	1.390
R_{9-10}	1.459	1.465	1.466
R_{10-11}	1.403	1.390	1.390
R_{11-12}	1.397	1.389	1.388
R_{12-13}	1.420	1.405	1.402
R_{13-14}	1.485	1.490	1.482
R_{14-15}	1.419	1.403	1.399
R_{15-16}	1.394	1.387	1.387
R_{16-17}	1.408	1.393	1.393
R_{17-18}	1.481	1.479	1.476
Bond Angle (A)			
A_{1-2-3}	121.2	120.5	120.3
A_{2-3-4}	120.4	120.2	120.1
A_{3-4-5}	121.5	121.2	121.0
A_{4-5-6}	121.4	121.1	120.9
A_{5-6-7}	120.6	120.5	120.3
A_{6-7-8}	121.9	121.7	121.5
A_{7-8-9}	119.0	119.0	119.0
A_{8-9-10}	131.1	131.2	131.3
$A_{9-10-11}$	131.1	131.3	131.3
$A_{10-11-12}$	119.0	119.0	119.0
$A_{11-12-13}$	122.0	121.9	121.5
$A_{12-13-14}$	120.7	120.7	120.7
$A_{13-14-15}$	121.3	121.2	120.8
$A_{14-15-16}$	121.2	121.2	120.7
$A_{15-16-17}$	120.7	120.5	120.4
$A_{16-17-18}$	119.9	120.1	120.2
Dihedral Angle (D_h)			
$D_{1-2-3-4}$	178.8	178.7	179.1

Table S7 (continued):

$D_{2\text{-}3\text{-}4\text{-}5}$	1.2	0.9	0.3
$D_{3\text{-}4\text{-}5\text{-}6}$	179.2	179.6	178.0
$D_{4\text{-}5\text{-}6\text{-}7}$	20.9	26.1	35.7
$D_{5\text{-}6\text{-}7\text{-}8}$	179.6	179.8	178.8
$D_{6\text{-}7\text{-}8\text{-}9}$	1.1	1.2	0.1
$D_{7\text{-}8\text{-}9\text{-}10}$	178.1	177.9	179.8
$D_{8\text{-}9\text{-}10\text{-}11}$	0.3	0.7	0.1
$D_{9\text{-}10\text{-}11\text{-}12}$	178.5	177.7	179.9
$D_{10\text{-}11\text{-}12\text{-}13}$	1.4	1.5	0.1
$D_{11\text{-}12\text{-}13\text{-}14}$	178.9	179.3	179.6
$D_{12\text{-}13\text{-}14\text{-}15}$	18.5	16.8	37.1
$D_{13\text{-}14\text{-}15\text{-}16}$	179.9	179.1	178.9
$D_{14\text{-}15\text{-}16\text{-}17}$	1.7	1.4	0.0
$D_{15\text{-}16\text{-}17\text{-}18}$	176.9	176.7	179.1

Table S8. Selected bond lengths (R) (in Å), bond angles (A) (in degrees), and dihedral angles (D_h) (in degrees) of DPF-DTF without SCs interacting with (6,5) SWCNT. The labeling of atoms is shown in Figure 1.

Bond Length (R)	**B97D**	**wB97XD**	**CAM-B3LYP**
R_{1-2}	1.453	1.463	1.461
R_{2-3}	1.420	1.403	1.402
R_{3-4}	1.395	1.388	1.387
R_{4-5}	1.415	1.399	1.397
R_{5-6}	1.480	1.485	1.482
R_{6-7}	1.419	1.404	1.402
R_{7-8}	1.398	1.392	1.389
R_{8-9}	1.404	1.391	1.390
R_{9-10}	1.461	1.469	1.466
R_{10-11}	1.403	1.391	1.389
R_{11-12}	1.398	1.392	1.389
R_{12-13}	1.419	1.404	1.401
R_{13-14}	1.479	1.485	1.482
R_{14-15}	1.417	1.401	1.400
R_{15-16}	1.391	1.385	1.383
R_{16-17}	1.421	1.406	1.404
R_{17-18}	1.455	1.462	1.461
Bond Angle (A)			
A_{1-2-3}	126.4	125.1	125.5
A_{2-3-4}	121.3	121.2	121.1
A_{3-4-5}	122.0	121.8	121.6
A_{4-5-6}	122.1	121.7	121.5
A_{5-6-7}	120.9	121.2	120.7
A_{6-7-8}	121.9	121.8	121.6
A_{7-8-9}	119.1	119.1	119.0
A_{8-9-10}	131.5	131.9	131.4
$A_{9-10-11}$	131.3	131.9	131.3
$A_{10-11-12}$	119.0	119.1	119.1
$A_{11-12-13}$	122.0	121.8	121.6
$A_{12-13-14}$	120.7	121.1	120.5
$A_{13-14-15}$	121.5	121.7	121.3
$A_{14-15-16}$	121.4	121.2	121.1
$A_{15-16-17}$	121.8	121.9	121.7
$A_{16-17-18}$	117.8	117.4	117.7
Dihedral Angle (D_h)			
$D_{1-2-3-4}$	176.4	179.2	179.7

Table S8 (continued):

$D_{2\text{-}3\text{-}4\text{-}5}$	0.3	0.4	0.2
$D_{3\text{-}4\text{-}5\text{-}6}$	176.8	179.2	179.8
$D_{4\text{-}5\text{-}6\text{-}7}$	26.1	26.4	37.8
$D_{5\text{-}6\text{-}7\text{-}8}$	176.3	179.8	179.3
$D_{6\text{-}7\text{-}8\text{-}9}$	0.1	1.0	0.1
$D_{7\text{-}8\text{-}9\text{-}10}$	178.0	178.8	179.7
$D_{8\text{-}9\text{-}10\text{-}11}$	0.9	1.1	1.4
$D_{9\text{-}10\text{-}11\text{-}12}$	179.1	178.4	179.3
$D_{10\text{-}11\text{-}12\text{-}13}$	-0.5	0.6	0.1
$D_{11\text{-}12\text{-}13\text{-}14}$	179.5	178.0	179.2
$D_{12\text{-}13\text{-}14\text{-}15}$	24.5	27.6	36.5
$D_{13\text{-}14\text{-}15\text{-}16}$	179.0	177.9	179.9
$D_{14\text{-}15\text{-}16\text{-}17}$	0.9	0.8	0.3
$D_{15\text{-}16\text{-}17\text{-}18}$	179.5	179.0	180.0

Table S9. Selected bond lengths (R) (in Å), bond angles (A) (in degrees), and dihedral angles (D_h) (in degrees) of DPF-ALD with 2 SCs interacting with (6,5) SWCNT. The labeling of atoms is shown in Figure 1.

Bond Length (R)	**B97D**	**wB97XD**	**CAM-B3LYP**
R_{1-2}	1.482	1.480	1.476
R_{2-3}	1.413	1.398	1.396
R_{3-4}	1.395	1.387	1.383
R_{4-5}	1.418	1.402	1.403
R_{5-6}	1.482	1.485	1.482
R_{6-7}	1.419	1.403	1.401
R_{7-8}	1.406	1.396	1.389
R_{8-9}	1.408	1.393	1.389
R_{9-10}	1.477	1.480	1.466
R_{10-11}	1.408	1.393	1.389
R_{11-12}	1.406	1.396	1.389
R_{12-13}	1.420	1.404	1.401
R_{13-14}	1.482	1.484	1.482
R_{14-15}	1.415	1.399	1.400
R_{15-16}	1.398	1.389	1.386
R_{16-17}	1.411	1.396	1.393
R_{17-18}	1.479	1.477	1.475
Bond Angle (A)			
A_{1-2-3}	121.4	120.7	120.3
A_{2-3-4}	120.3	120.2	120.1
A_{3-4-5}	120.9	120.8	120.9
A_{4-5-6}	121.7	121.5	120.8
A_{5-6-7}	123.2	123.1	120.5
A_{6-7-8}	121.8	121.6	121.3
A_{7-8-9}	119.3	119.3	119.0
A_{8-9-10}	133.8	133.4	131.3
$A_{9-10-11}$	133.8	133.4	131.2
$A_{10-11-12}$	119.3	119.3	119.0
$A_{11-12-13}$	121.9	121.6	121.4
$A_{12-13-14}$	123.1	123.0	120.3
$A_{13-14-15}$	121.6	121.7	120.6
$A_{14-15-16}$	120.7	120.5	120.7
$A_{15-16-17}$	120.7	120.4	120.4
$A_{16-17-18}$	120.0	120.1	120.0
Dihedral Angle (D_h)			
$D_{1-2-3-4}$	-178.7	-178.0	-180.0

Table S9 (continued):

$D_{2\text{-}3\text{-}4\text{-}5}$	0.7	0.1	-0.1
$D_{3\text{-}4\text{-}5\text{-}6}$	175.6	175.5	-180.0
$D_{4\text{-}5\text{-}6\text{-}7}$	34.6	39.3	38.2
$D_{5\text{-}6\text{-}7\text{-}8}$	-179.4	-178.9	180.0
$D_{6\text{-}7\text{-}8\text{-}9}$	0.4	0.0	0.1
$D_{7\text{-}8\text{-}9\text{-}10}$	179.1	179.5	179.7
$D_{8\text{-}9\text{-}10\text{-}11}$	0.7	1.3	0.2
$D_{9\text{-}10\text{-}11\text{-}12}$	-179.6	179.0	-179.7
$D_{10\text{-}11\text{-}12\text{-}13}$	0.0	0.3	0.1
$D_{11\text{-}12\text{-}13\text{-}14}$	178.9	-179.4	179.8
$D_{12\text{-}13\text{-}14\text{-}15}$	-31.3	-38.4	-37.0
$D_{13\text{-}14\text{-}15\text{-}16}$	-175.8	-177.2	179.4
$D_{14\text{-}15\text{-}16\text{-}17}$	0.1	0.0	0.2
$D_{15\text{-}16\text{-}17\text{-}18}$	177.9	179.8	-179.9

Table S10. Selected bond lengths (R) (in Å), bond angles (A) (in degrees), and dihedral angles (D_h) (in degrees) of DPF-ALD with 6 SCs interacting with (6,5) SWCNT. The labeling of atoms is shown in Figure 1.

Bond Length (R)	**B97D**	**wB97XD**	**CAM-B3LYP**
R_{1-2}	1.480	1.478	1.475
R_{2-3}	1.414	1.407	1.405
R_{3-4}	1.399	1.400	1.396
R_{4-5}	1.424	1.390	1.395
R_{5-6}	1.485	1.489	1.485
R_{6-7}	1.417	1.399	1.401
R_{7-8}	1.405	1.397	1.390
R_{8-9}	1.408	1.391	1.389
R_{9-10}	1.472	1.478	1.468
R_{10-11}	1.405	1.393	1.390
R_{11-12}	1.406	1.395	1.390
R_{12-13}	1.413	1.402	1.402
R_{13-14}	1.484	1.484	1.486
R_{14-15}	1.404	1.405	1.409
R_{15-16}	1.407	1.389	1.387
R_{16-17}	1.421	1.398	1.398
R_{17-18}	1.480	1.478	1.475
Bond Angle (A)			
A_{1-2-3}	118.8	124.0	124.2
A_{2-3-4}	122.0	118.6	118.6
A_{3-4-5}	119.3	121.4	122.4
A_{4-5-6}	125.1	121.6	119.1
A_{5-6-7}	123.1	122.0	119.7
A_{6-7-8}	121.1	121.2	121.5
A_{7-8-9}	119.3	119.0	118.9
A_{8-9-10}	132.5	132.7	131.4
$A_{9-10-11}$	132.4	132.9	131.9
$A_{10-11-12}$	119.0	119.4	119.4
$A_{11-12-13}$	121.1	121.2	121.3
$A_{12-13-14}$	122.0	123.8	122.9
$A_{13-14-15}$	119.7	122.7	123.5
$A_{14-15-16}$	121.6	119.7	119.2
$A_{15-16-17}$	119.0	122.2	122.4
$A_{16-17-18}$	122.1	117.0	116.9
Dihedral Angle (D_h)			
$D_{1-2-3-4}$	179.1	179.4	177.7

Table S10 (continued):

$D_{2\text{-}3\text{-}4\text{-}5}$	1.2	2.3	0.4
$D_{3\text{-}4\text{-}5\text{-}6}$	179.9	178.9	179.8
$D_{4\text{-}5\text{-}6\text{-}7}$	49.1	74.5	43.4
$D_{5\text{-}6\text{-}7\text{-}8}$	162.7	173.4	178.3
$D_{6\text{-}7\text{-}8\text{-}9}$	0.2	0.1	0.0
$D_{7\text{-}8\text{-}9\text{-}10}$	164.7	175.1	179.3
$D_{8\text{-}9\text{-}10\text{-}11}$	4.3	0.7	1.2
$D_{9\text{-}10\text{-}11\text{-}12}$	170.1	178.4	179.3
$D_{10\text{-}11\text{-}12\text{-}13}$	1.4	0.2	0.4
$D_{11\text{-}12\text{-}13\text{-}14}$	176.0	179.3	178.9
$D_{12\text{-}13\text{-}14\text{-}15}$	58.6	47.6	38.6
$D_{13\text{-}14\text{-}15\text{-}16}$	176.4	173.4	177.3
$D_{14\text{-}15\text{-}16\text{-}17}$	1.6	0.9	1.2
$D_{15\text{-}16\text{-}17\text{-}18}$	175.6	177.4	178.9

Table S11. Selected bond lengths (R) (in Å), bond angles (A) (in degrees), and dihedral angles (D_h) (in degrees) of DPF-DTF with 6 SCs interacting with (6,5) SWCNT. The labeling of atoms is shown in Figure 1.

Bond Length (R)	**B97D**	**wB97XD**	**CAM-B3LYP**
R_{1-2}	1.454	1.459	1.462
R_{2-3}	1.419	1.401	1.401
R_{3-4}	1.396	1.389	1.388
R_{4-5}	1.412	1.398	1.398
R_{5-6}	1.479	1.482	1.482
R_{6-7}	1.417	1.403	1.402
R_{7-8}	1.403	1.390	1.390
R_{8-9}	1.405	1.389	1.390
R_{9-10}	1.469	1.466	1.468
R_{10-11}	1.406	1.391	1.391
R_{11-12}	1.404	1.391	1.391
R_{12-13}	1.417	1.403	1.401
R_{13-14}	1.481	1.482	1.482
R_{14-15}	1.415	1.402	1.400
R_{15-16}	1.399	1.386	1.385
R_{16-17}	1.415	1.403	1.402
R_{17-18}	1.472	1.464	1.466
Bond Angle (A)			
A_{1-2-3}	125.8	123.9	124.5
A_{2-3-4}	121.2	120.6	121.1
A_{3-4-5}	121.5	121.4	121.5
A_{4-5-6}	121.7	120.7	121.5
A_{5-6-7}	121.4	119.0	120.4
A_{6-7-8}	121.6	121.6	121.5
A_{7-8-9}	119.1	118.7	119.0
A_{8-9-10}	132.4	131.0	131.5
$A_{9-10-11}$	132.7	131.5	131.6
$A_{10-11-12}$	119.2	119.0	119.1
$A_{11-12-13}$	121.7	121.1	121.4
$A_{12-13-14}$	122.9	120.0	121.3
$A_{13-14-15}$	122.3	121.3	121.1
$A_{14-15-16}$	121.2	120.9	121.2
$A_{15-16-17}$	120.9	121.5	121.3
$A_{16-17-18}$	121.8	118.3	118.7
Dihedral Angle (D_h)			
$D_{1-2-3-4}$	-177.4	175.8	177.1

Table S11 (continued):

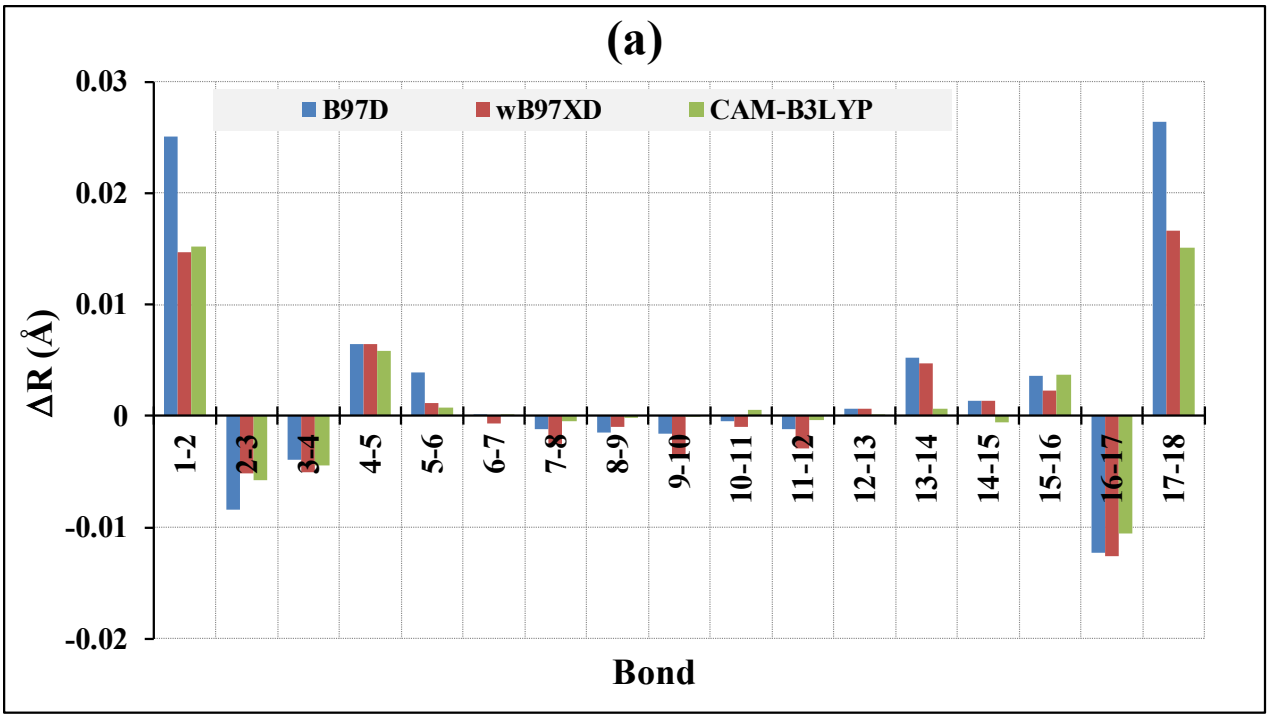
$D_{2\text{-}3\text{-}4\text{-}5}$	0.8	1.1	0.2
$D_{3\text{-}4\text{-}5\text{-}6}$	178.4	-174.1	-177.3
$D_{4\text{-}5\text{-}6\text{-}7}$	42.7	41.0	35.1
$D_{5\text{-}6\text{-}7\text{-}8}$	177.6	175.5	178.4
$D_{6\text{-}7\text{-}8\text{-}9}$	0.9	-0.5	-0.5
$D_{7\text{-}8\text{-}9\text{-}10}$	-178.3	-177.7	-178.2
$D_{8\text{-}9\text{-}10\text{-}11}$	2.5	-1.1	-0.3
$D_{9\text{-}10\text{-}11\text{-}12}$	176.8	179.5	177.7
$D_{10\text{-}11\text{-}12\text{-}13}$	-0.1	-0.6	-0.5
$D_{11\text{-}12\text{-}13\text{-}14}$	-176.2	-179.1	-176.8
$D_{12\text{-}13\text{-}14\text{-}15}$	30.8	37.3	32.9
$D_{13\text{-}14\text{-}15\text{-}16}$	171.8	-177.6	178.3
$D_{14\text{-}15\text{-}16\text{-}17}$	-1.0	-0.9	-1.1
$D_{15\text{-}16\text{-}17\text{-}18}$	-172.3	179.5	-176.3

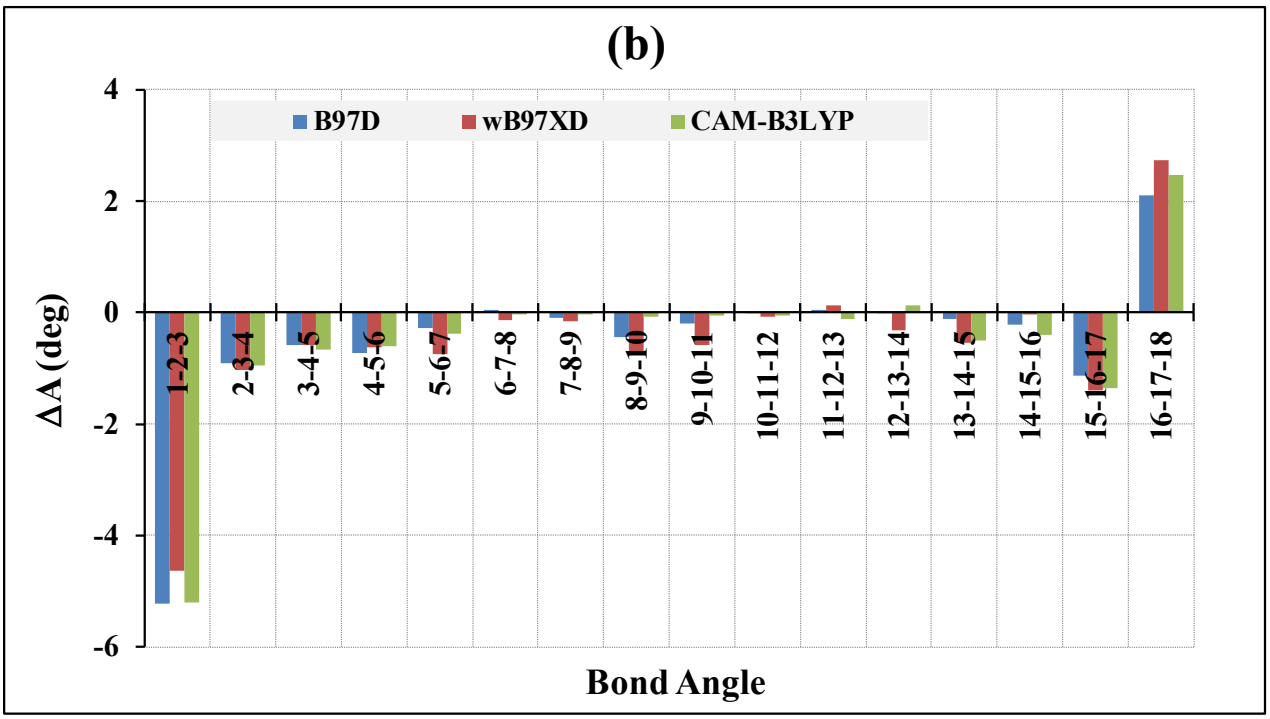
Table S12. Selected bond lengths (R) (in Å), bond angles (A) (in degrees), and dihedral angles (D_h) (in degrees) of DPF-DTF with 10 SCs interacting with (6,5) SWCNT. The labeling of atoms is shown in Figure 1.

Bond Length (R)	**B97D**	**wB97XD**	**CAM-B3LYP**
R_{1-2}	1.459	1.467	1.467
R_{2-3}	1.424	1.404	1.401
R_{3-4}	1.403	1.392	1.392
R_{4-5}	1.407	1.395	1.394
R_{5-6}	1.482	1.485	1.485
R_{6-7}	1.416	1.403	1.400
R_{7-8}	1.405	1.391	1.391
R_{8-9}	1.405	1.389	1.389
R_{9-10}	1.472	1.468	1.469
R_{10-11}	1.407	1.392	1.390
R_{11-12}	1.406	1.391	1.389
R_{12-13}	1.419	1.402	1.401
R_{13-14}	1.485	1.485	1.486
R_{14-15}	1.421	1.404	1.403
R_{15-16}	1.407	1.392	1.392
R_{16-17}	1.410	1.404	1.396
R_{17-18}	1.481	1.469	1.483
Bond Angle (A)			
A_{1-2-3}	126.4	123.4	124.3
A_{2-3-4}	120.2	119.8	119.9
A_{3-4-5}	122.6	122.0	122.2
A_{4-5-6}	119.9	119.5	119.4
A_{5-6-7}	121.1	118.2	119.8
A_{6-7-8}	121.7	121.7	121.5
A_{7-8-9}	119.1	118.7	119.0
A_{8-9-10}	132.9	131.3	131.6
$A_{9-10-11}$	133.5	131.6	131.7
$A_{10-11-12}$	119.7	119.1	119.3
$A_{11-12-13}$	121.5	121.0	121.3
$A_{12-13-14}$	125.5	121.5	121.8
$A_{13-14-15}$	124.9	124.9	123.1
$A_{14-15-16}$	119.6	119.4	119.6
$A_{15-16-17}$	122.3	122.6	121.9
$A_{16-17-18}$	120.5	117.7	119.8
Dihedral Angle (D_h)			
$D_{1-2-3-4}$	172.1	173.2	178.9

Table S12 (continued):

$D_{2\text{-}3\text{-}4\text{-}5}$	0.2	2.5	2.4
$D_{3\text{-}4\text{-}5\text{-}6}$	179.1	171.4	179.7
$D_{4\text{-}5\text{-}6\text{-}7}$	47.0	45.7	46.9
$D_{5\text{-}6\text{-}7\text{-}8}$	177.8	178.4	178.2
$D_{6\text{-}7\text{-}8\text{-}9}$	0.4	0.1	0.3
$D_{7\text{-}8\text{-}9\text{-}10}$	176.6	179.5	179.3
$D_{8\text{-}9\text{-}10\text{-}11}$	0.4	1.7	0.0
$D_{9\text{-}10\text{-}11\text{-}12}$	178.2	174.3	177.6
$D_{10\text{-}11\text{-}12\text{-}13}$	0.5	0.2	0.2
$D_{11\text{-}12\text{-}13\text{-}14}$	179.5	166.8	174.2
$D_{12\text{-}13\text{-}14\text{-}15}$	40.0	49.6	49.1
$D_{13\text{-}14\text{-}15\text{-}16}$	167.8	176.1	179.9
$D_{14\text{-}15\text{-}16\text{-}17}$	1.0	0.4	0.5
$D_{15\text{-}16\text{-}17\text{-}18}$	172.5	177.2	176.4


(a)
B97D
wB97XD
CAM-B3LYP
0.03
0.02
0.01
0
-0.01
-0.02
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
4
2
0
-2
-4
-6
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

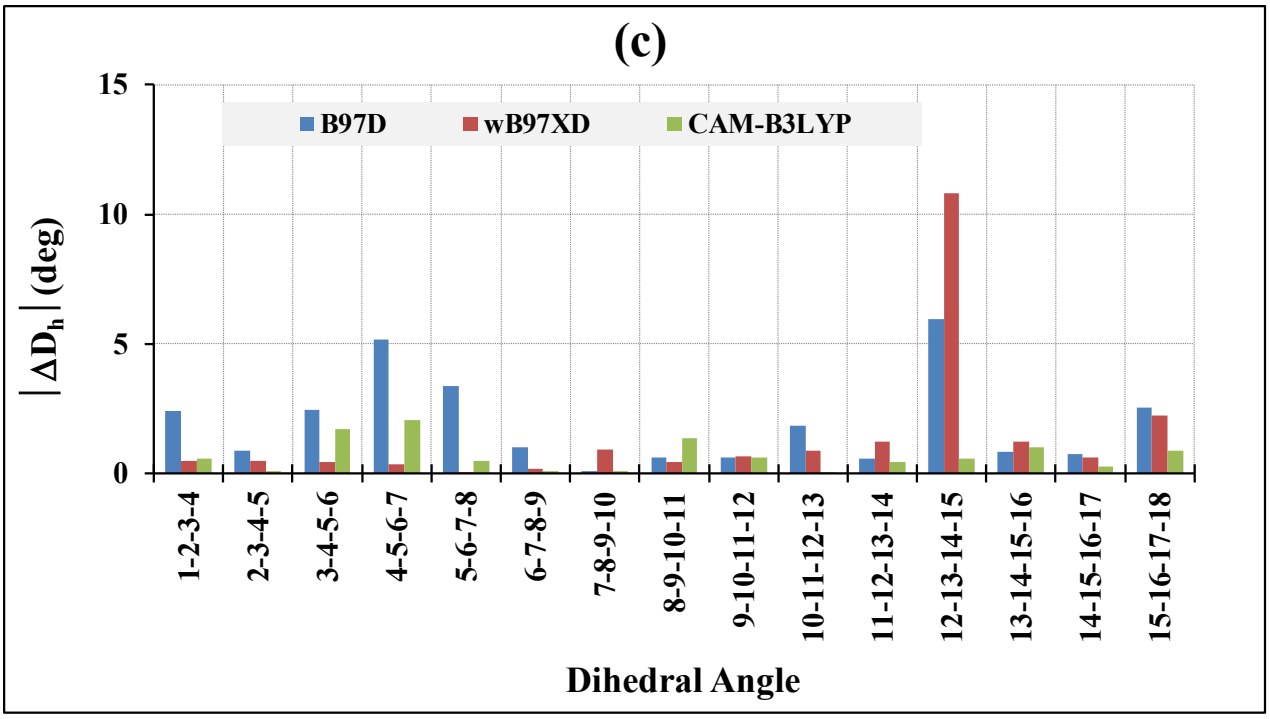
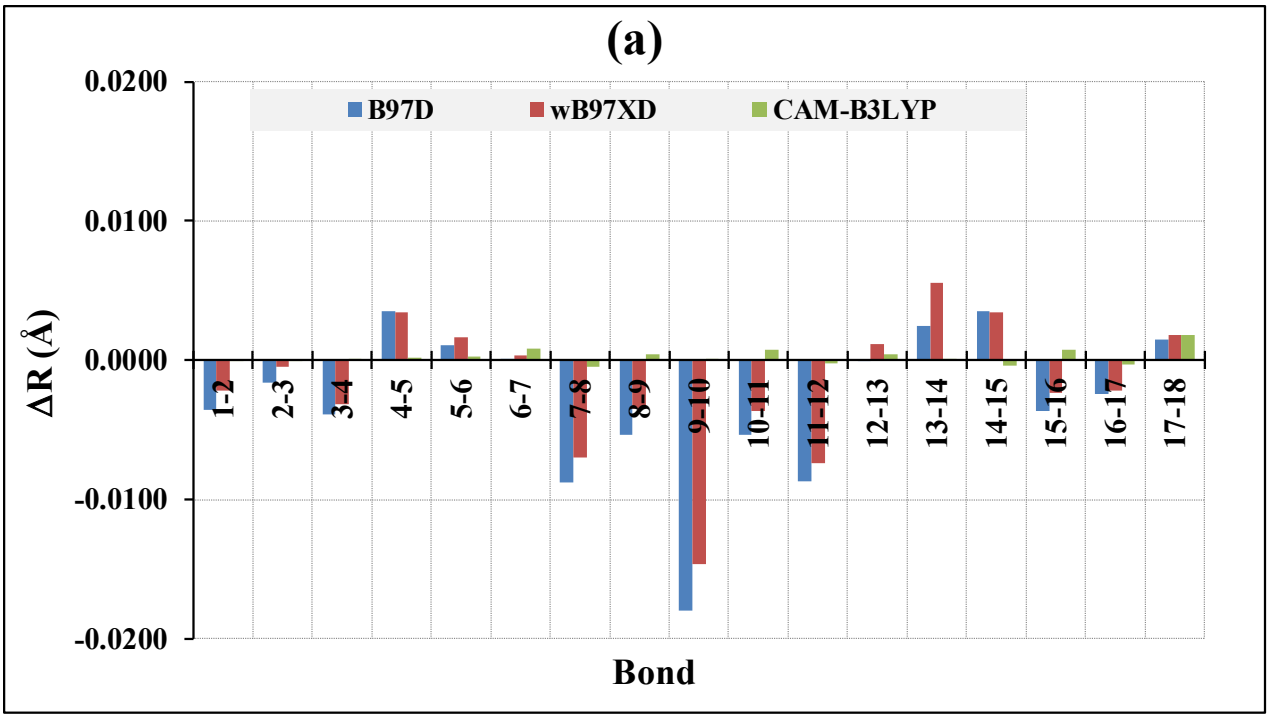
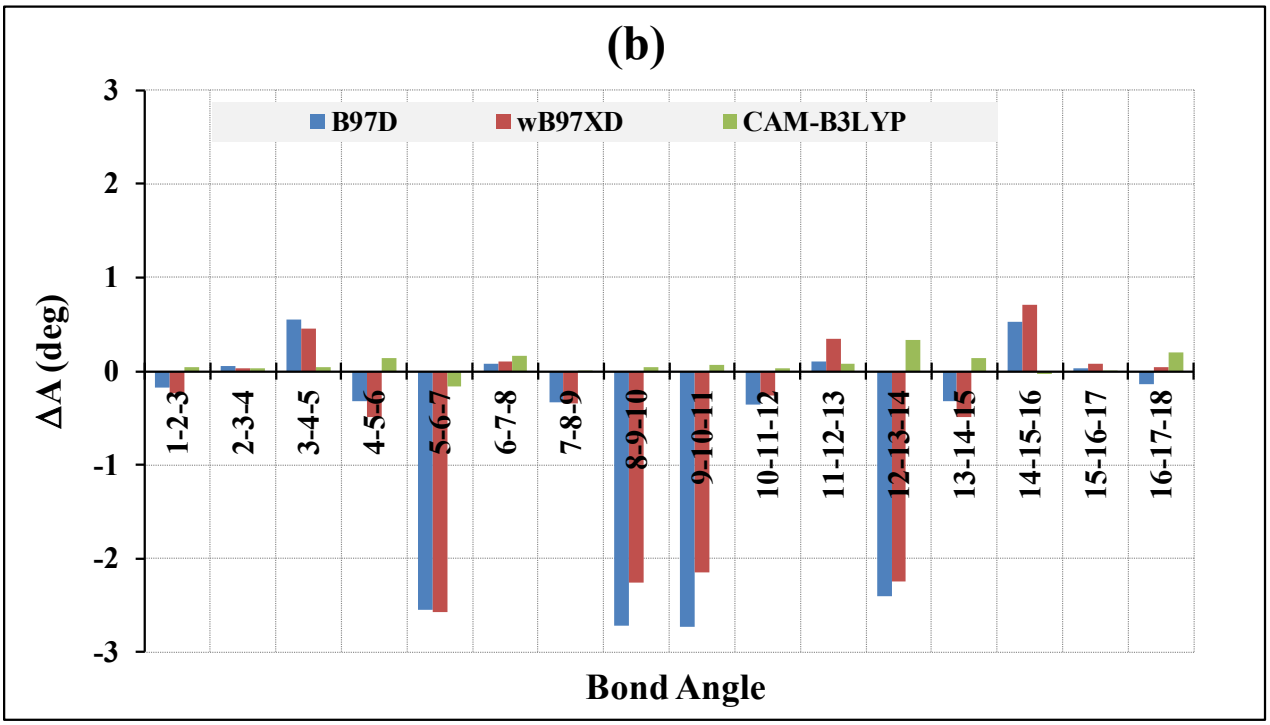


Figure S18. End group effect; differences between the geometrical parameters of the interacting DPF-ALD and DPF-DTF (without SCs) and (6,5) SWCNT obtained using B97D, wB97XD, and CAM-B3LYP methods with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1. This figure shows the differences between (a) bond lengths, (b) bond angles and (c) dihedral angles.


(a)
B97D
wB97XD
CAM-B3LYP
0.0200
0.0100
0.0000
-0.0100
-0.0200
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
3
2
1
0
-1
-2
-3
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

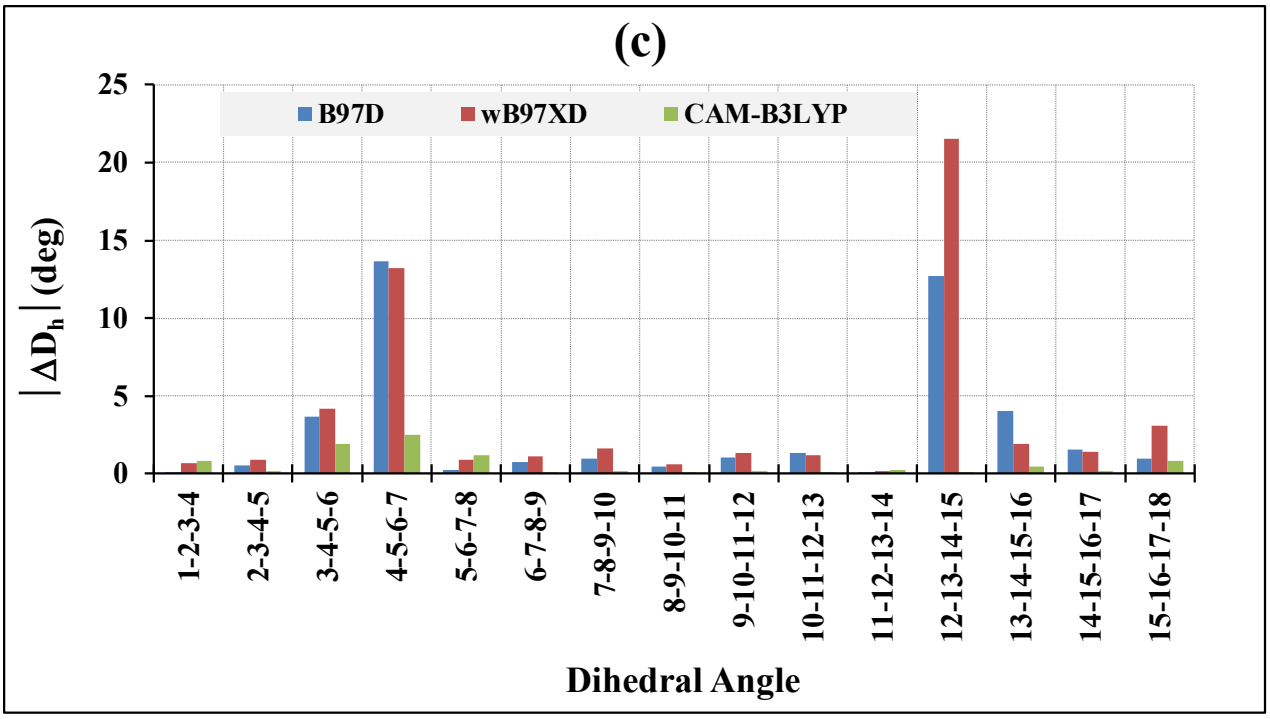
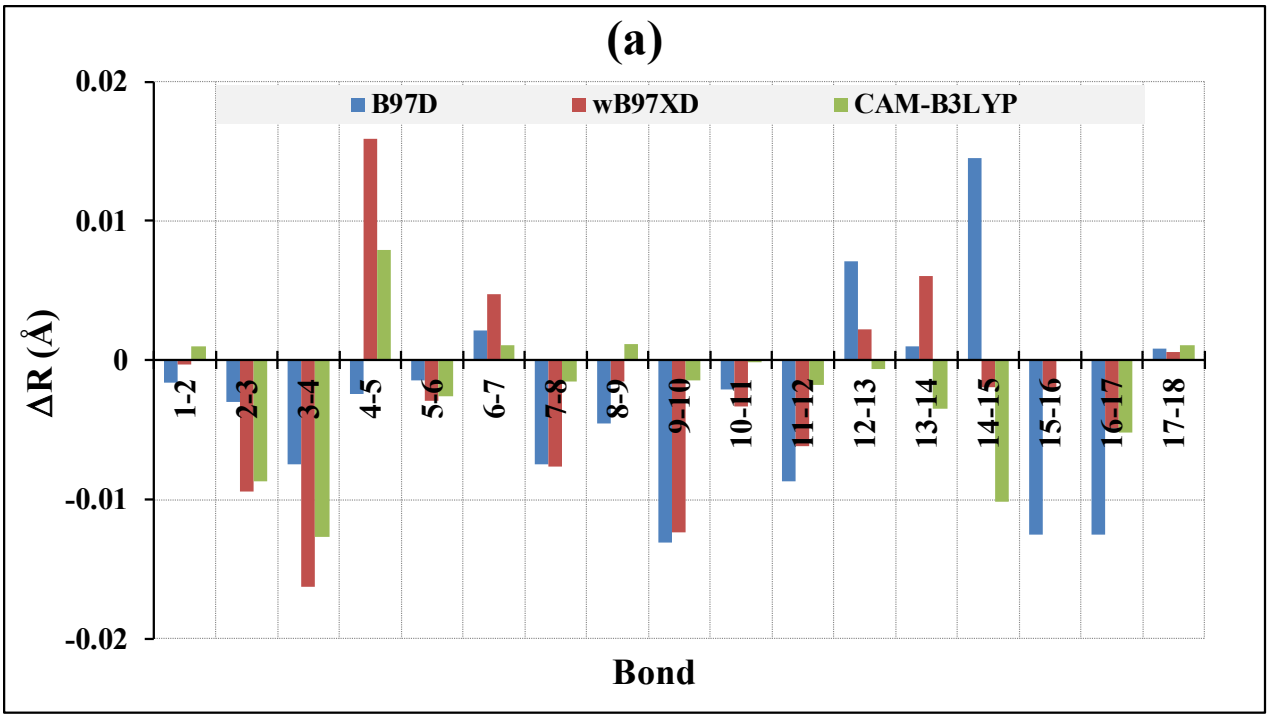
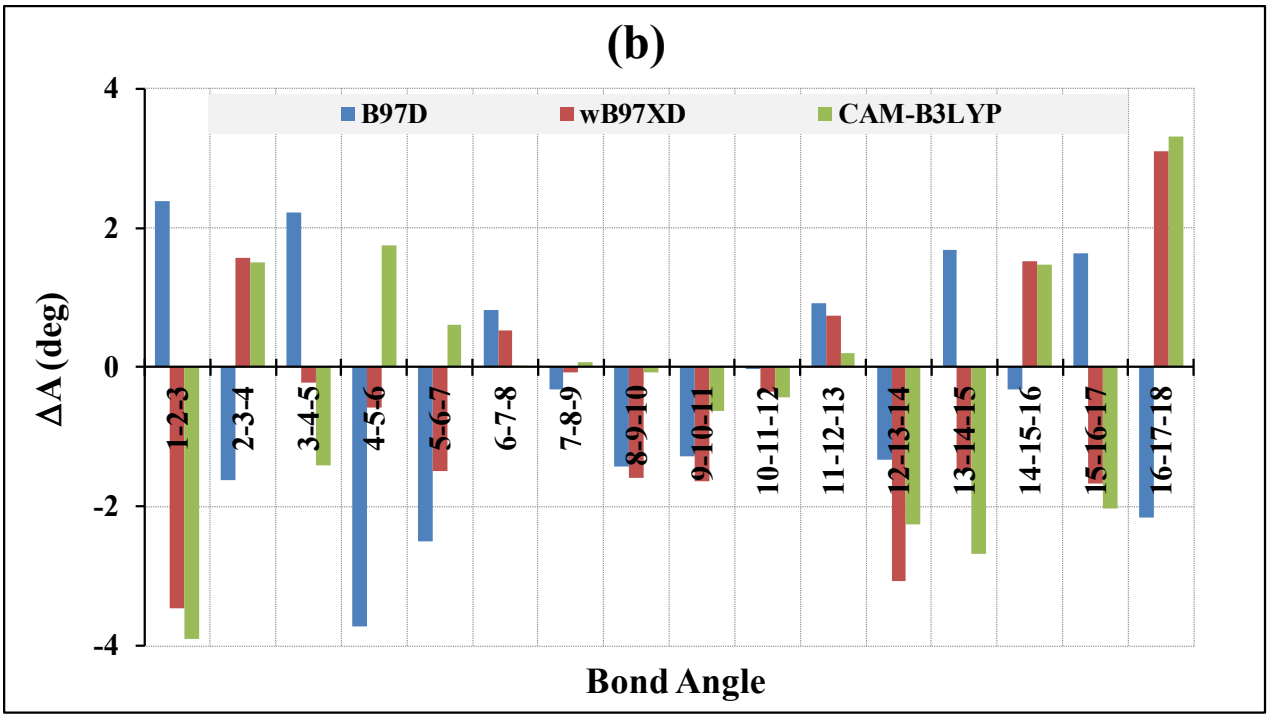


Figure S19. Side chain effect; differences between the geometrical parameters of the DPF-ALD with 2 SCs and DPF-ALD without SCs interacting with (6,5) SWCNT obtained using B97D, wB97XD, and CAM-B3LYP methods with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1. This figure shows the differences between (a) bond lengths, (b) bond angles and (c) dihedral angles.


(a)
B97D
wB97XD
CAM-B3LYP
0.02
0.01
0
-0.01
-0.02
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
4
2
0
-2
-4
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

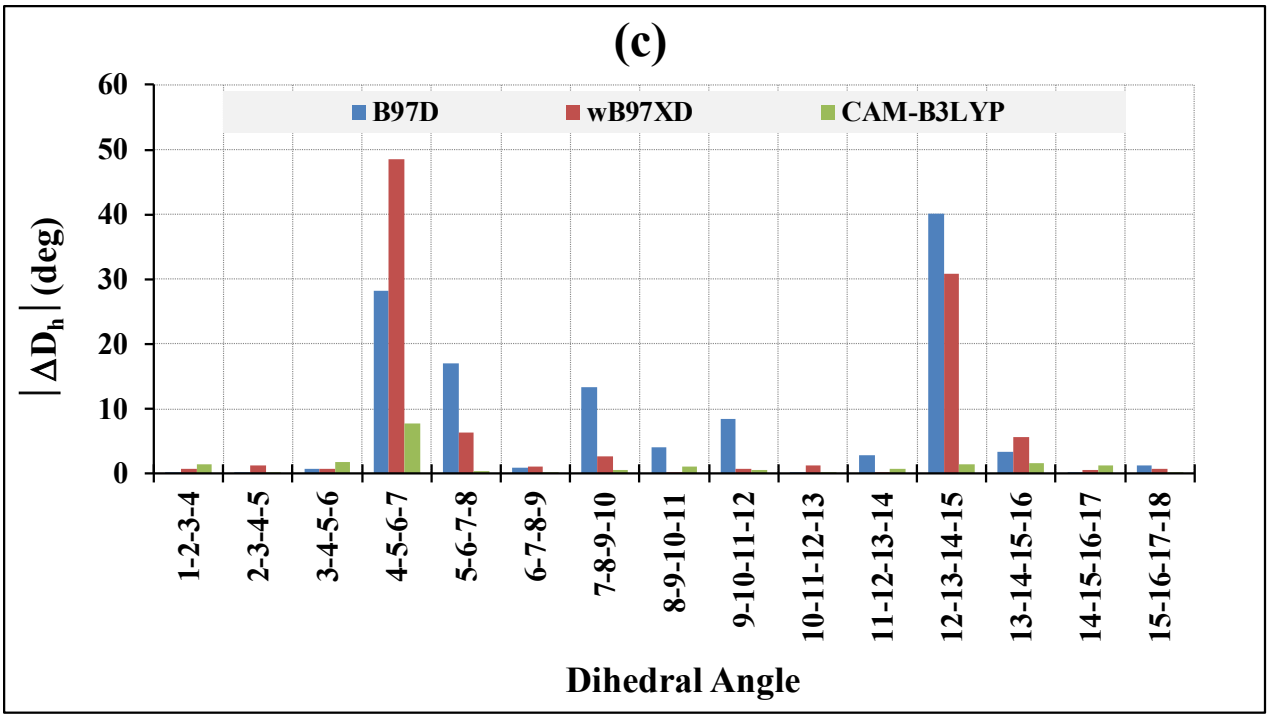
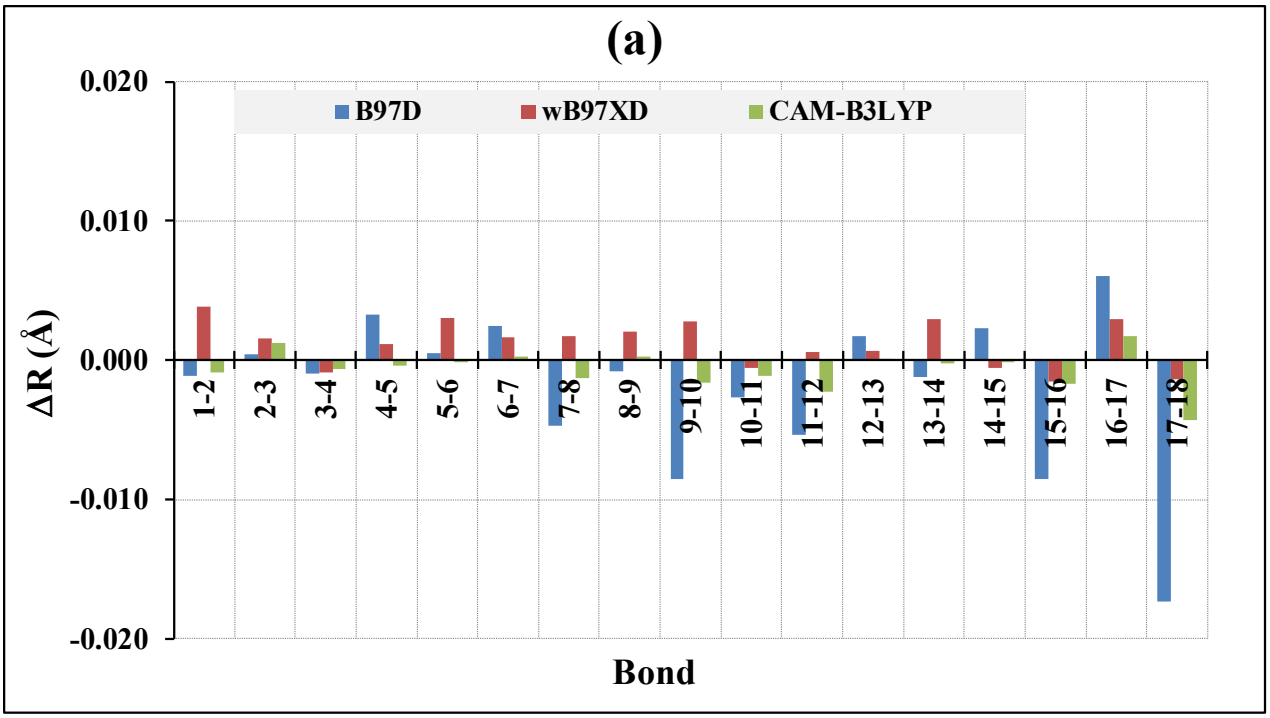
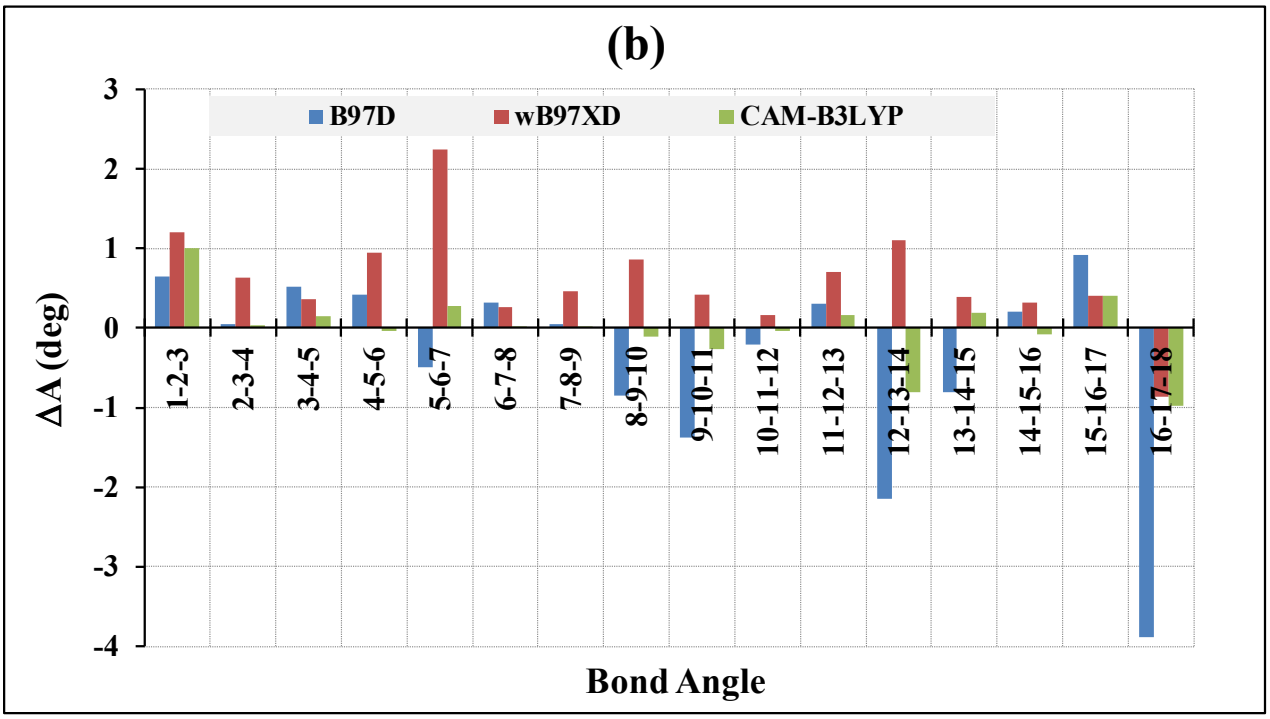


Figure S20. Side chain effect; differences between the geometrical parameters of the DPF-ALD with 6 SCs and DPF-ALD without SCs interacting with (6,5) SWCNT obtained using B97D, wB97XD, and CAM-B3LYP methods with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1. This figure shows the differences between (a) bond lengths, (b) bond angles and (c) dihedral angles.


(a)
B97D
wB97XD
CAM-B3LYP
0.020
0.010
0.000
-0.010
-0.020
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
3
2
1
0
-1
-2
-3
-4
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

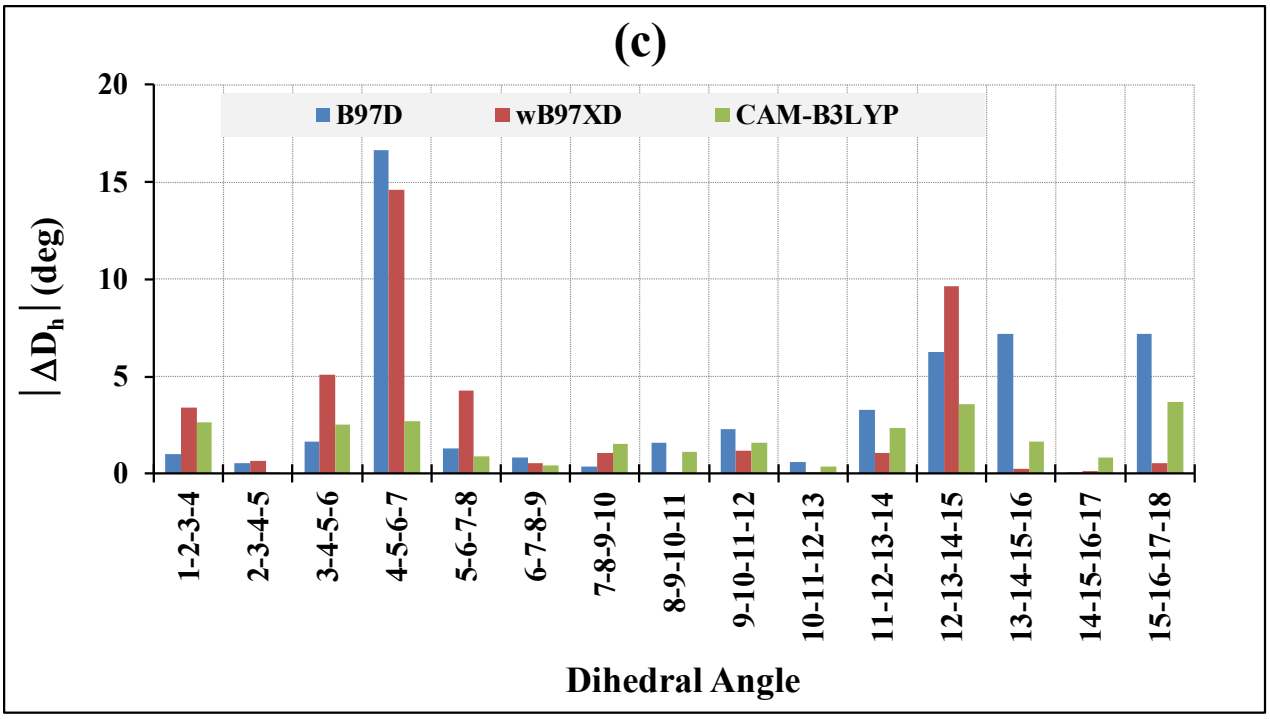
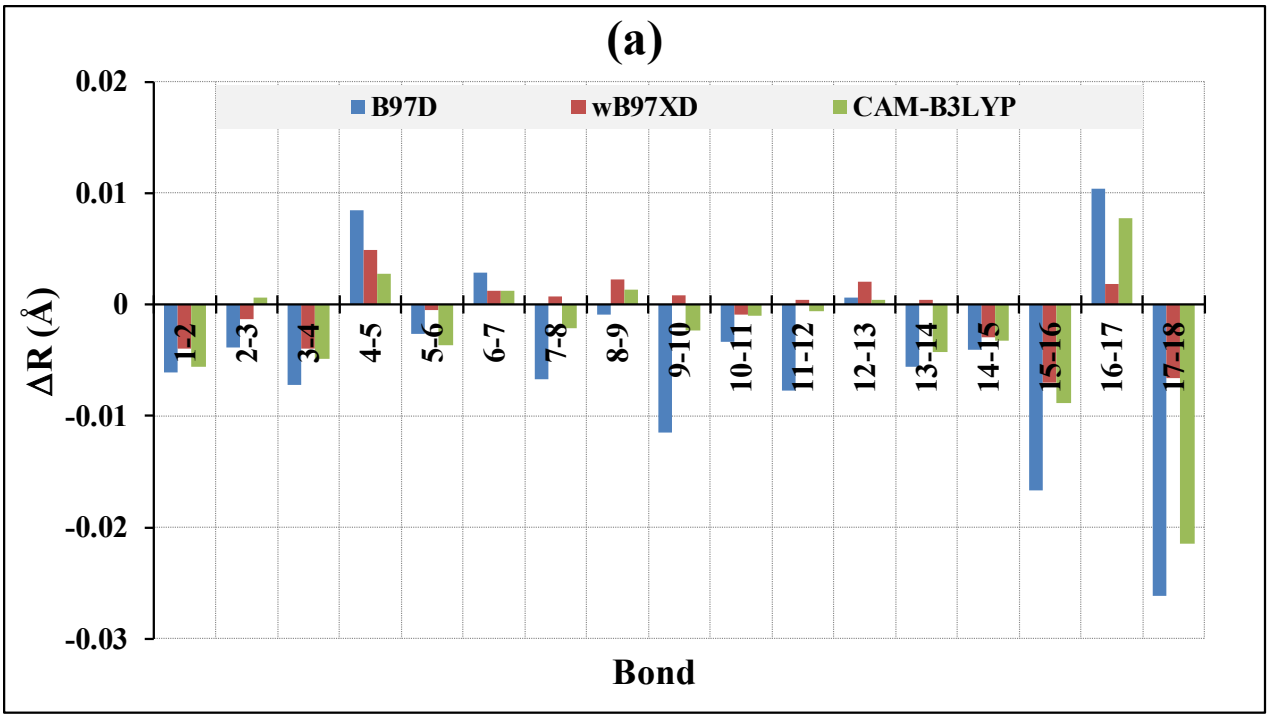
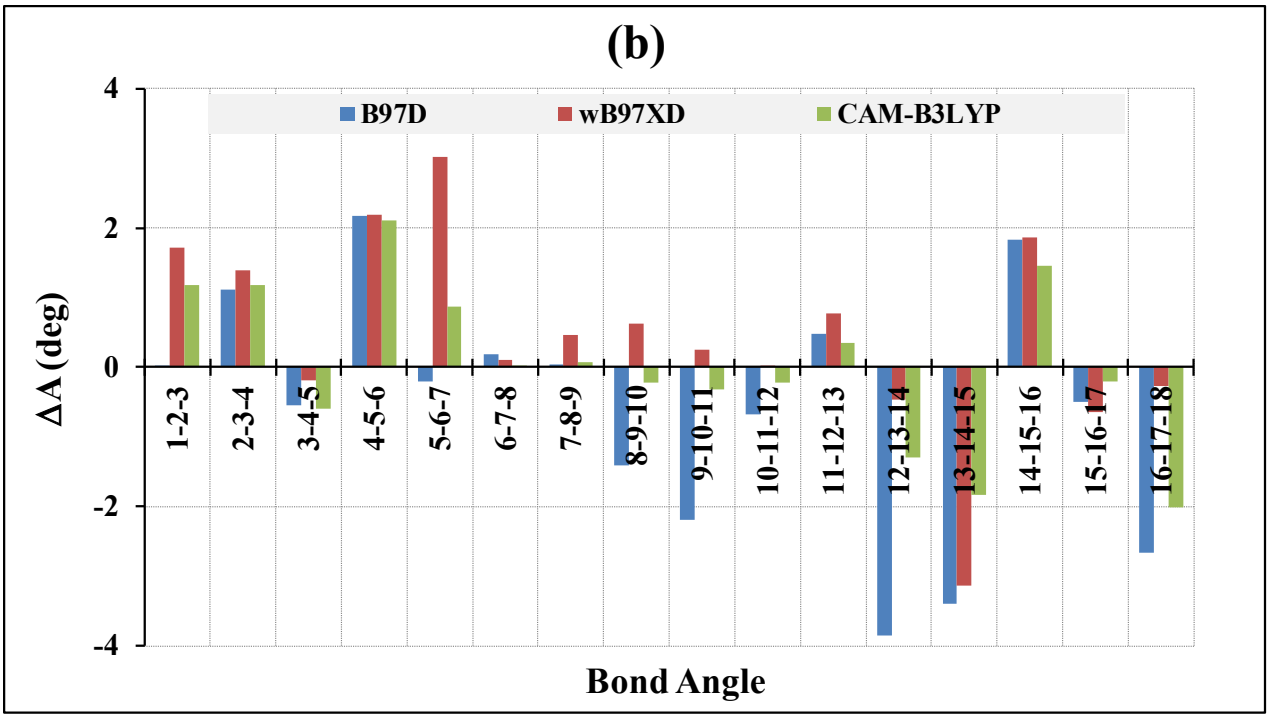


Figure S21. Side chain effect; differences between the geometrical parameters of the DPF-DTF with 6 SCs and DPF-DTF without SCs interacting with (6,5) SWCNT obtained using B97D, wB97XD, and CAM-B3LYP methods with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1. This figure shows the differences between (a) bond lengths, (b) bond angles and (c) dihedral angles.


(a)
B97D
wB97XD
CAM-B3LYP
0.02
0.01
0
-0.01
-0.02
-0.03
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
4
2
0
-2
-4
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

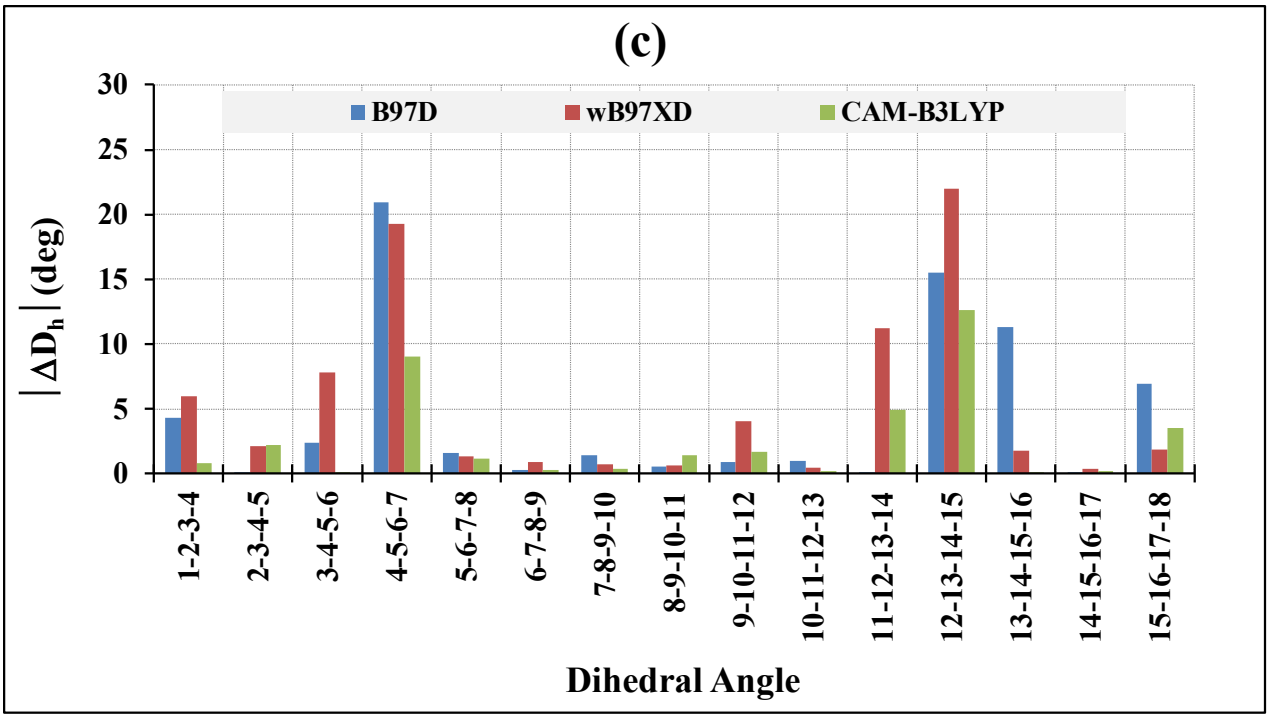
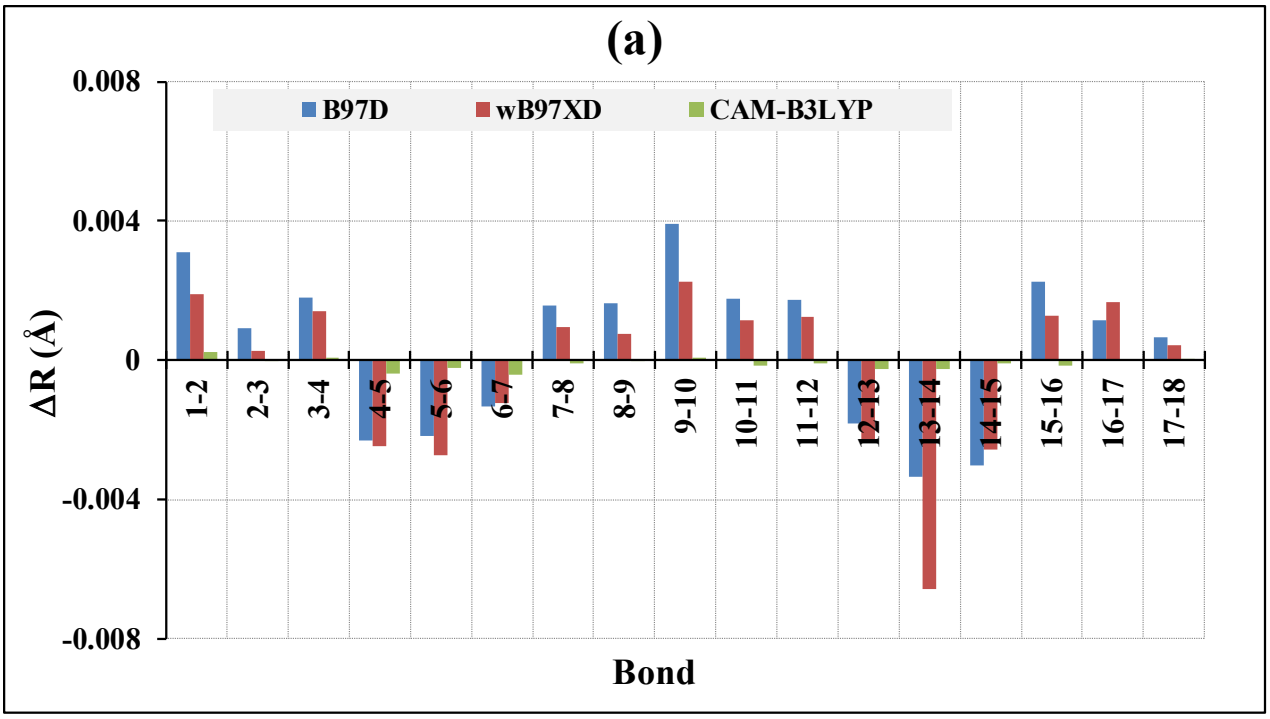
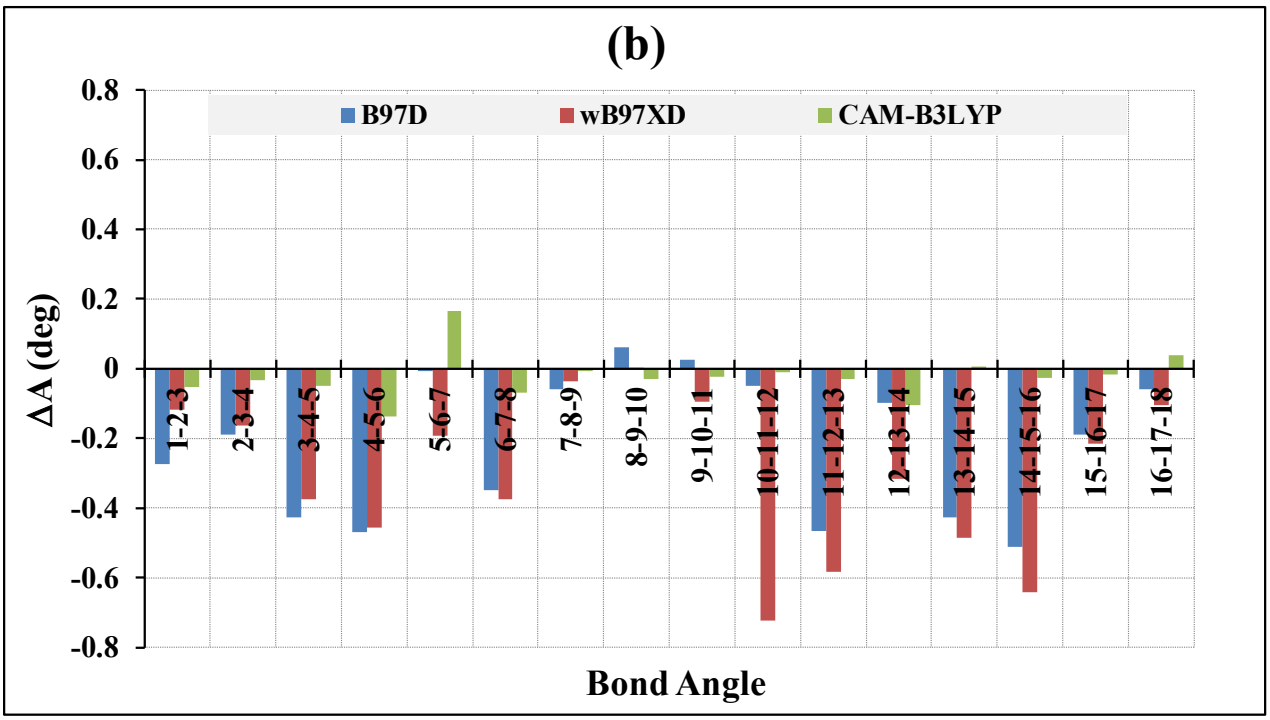


Figure S22. Side chain effect; differences between the geometrical parameters of the DPF-DTF with 10 SCs and DPF-DTF without SCs interacting with the (6,5) SWCNT obtained using B97D, wB97XD, and CAM-B3LYP methods with 6-31G(d) basis set. The labeling of atoms is shown in Figure 1. This figure shows the differences between (a) bond lengths, (b) bond angles and (c) dihedral angles.


(a)
B97D
wB97XD
CAM-B3LYP
0.008
0.004
0
-0.004
-0.008
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

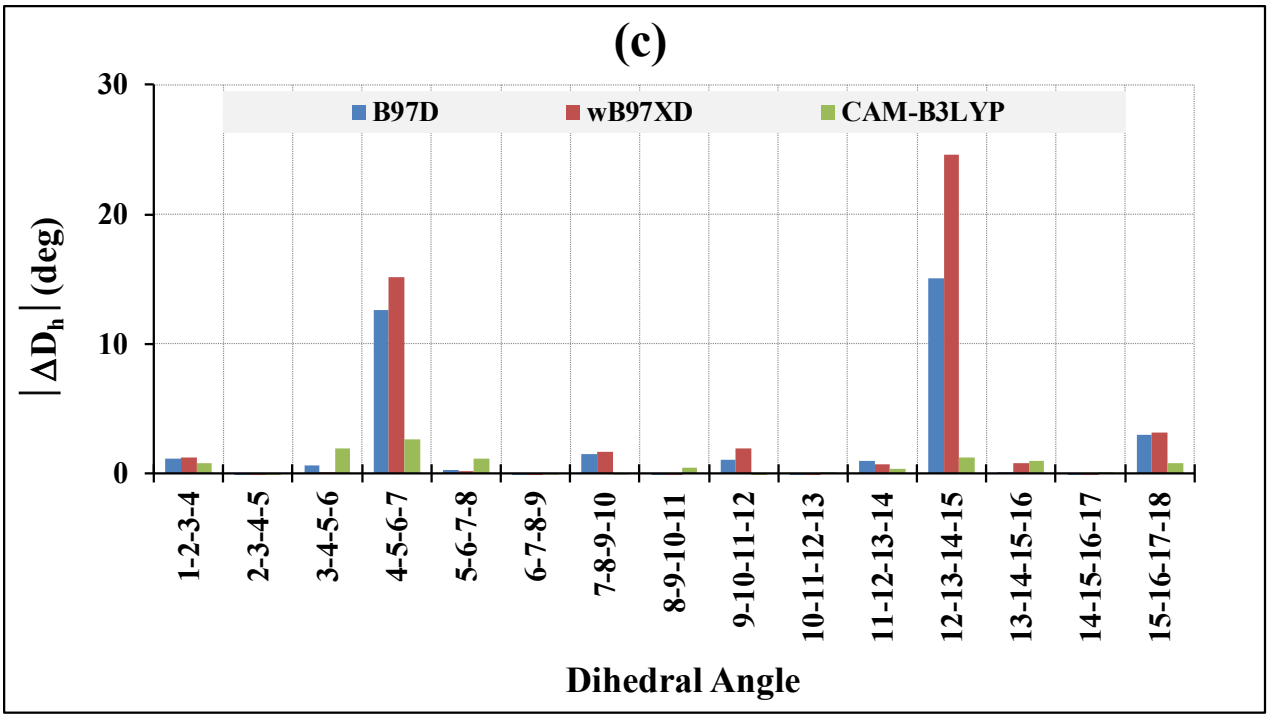
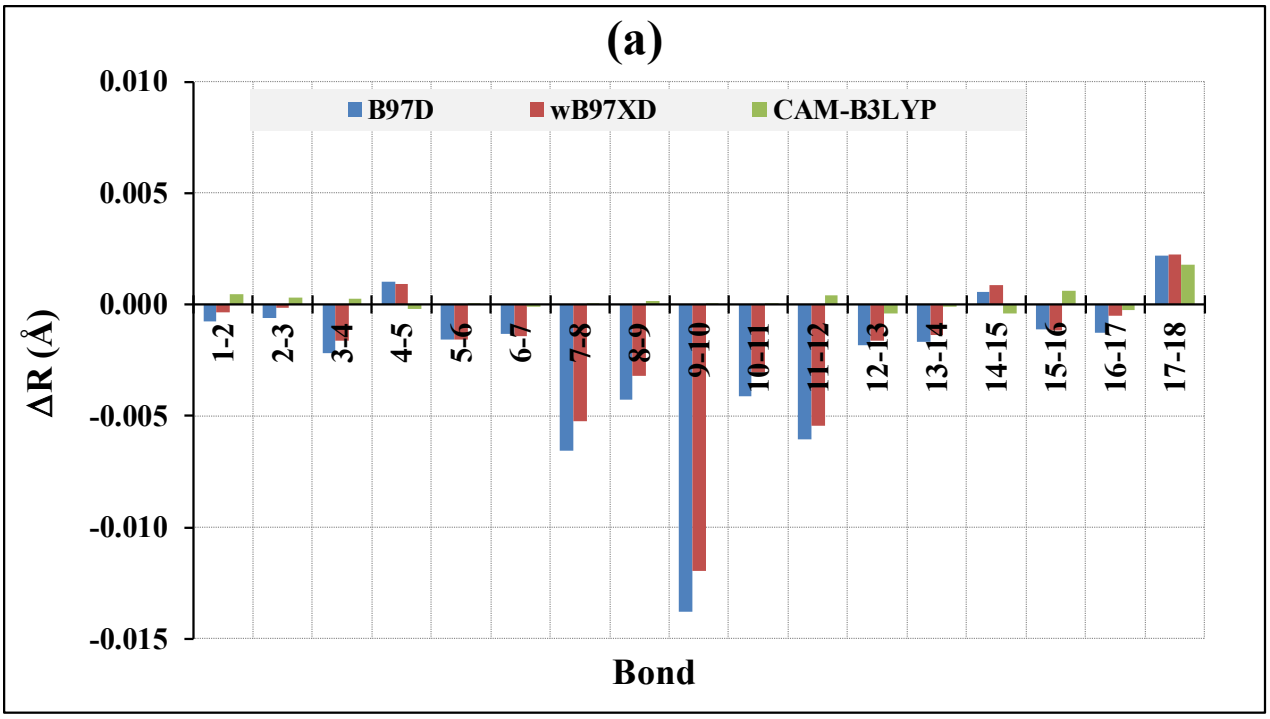
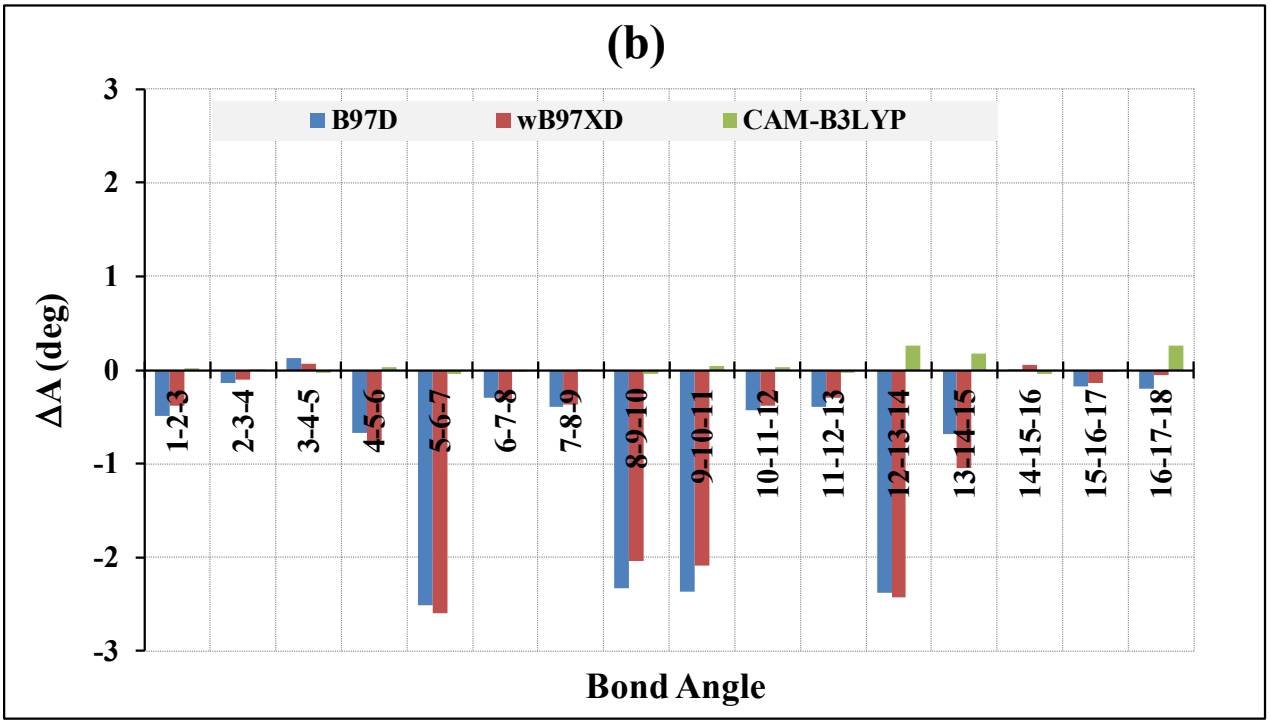


Figure S23. Dispersion effect on geometrical parameters of the DPF-ALD without SCs obtained using B97D, wB97XD, and CAM-B3LYP methods with 6-31G(d) basis set. This figure shows the effect on (a) bond lengths, (b) bond angles, and (c) dihedral angles. The labeling of atoms is shown in Figure 1.


(a)
B97D
wB97XD
CAM-B3LYP
0.010
0.005
0.000
-0.005
-0.010
-0.015
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
3
2
1
0
-1
-2
-3
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

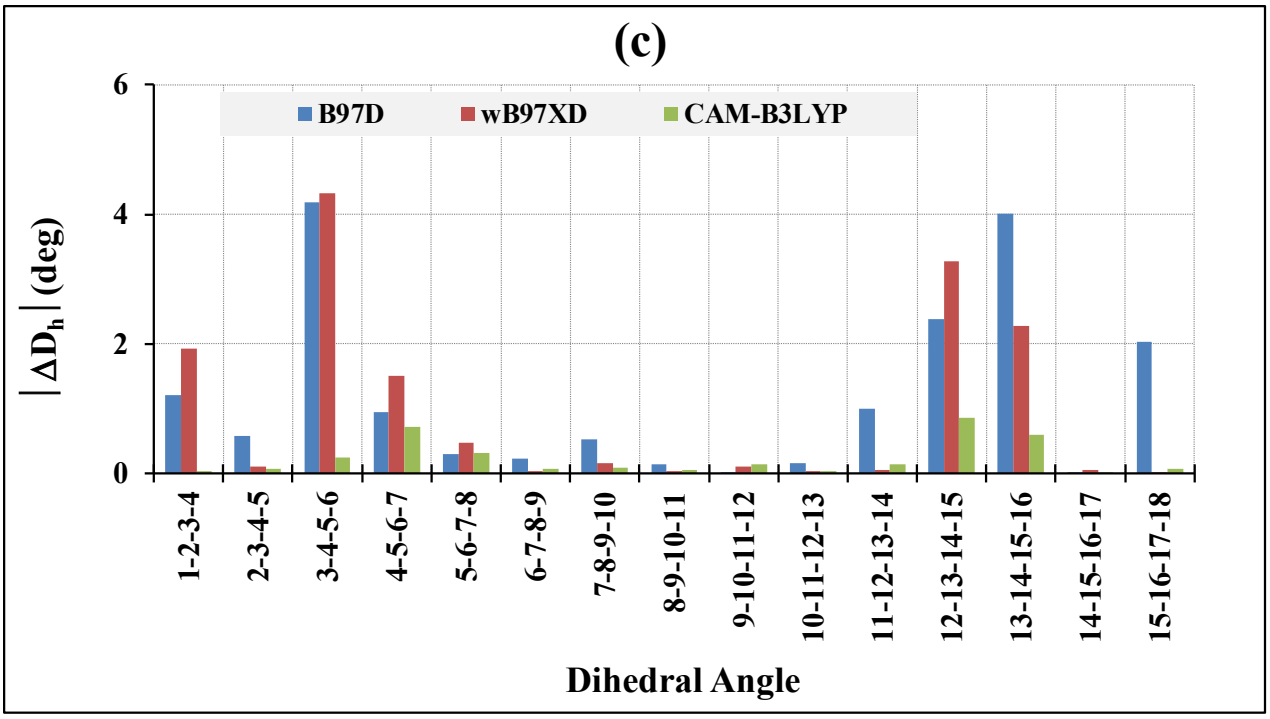
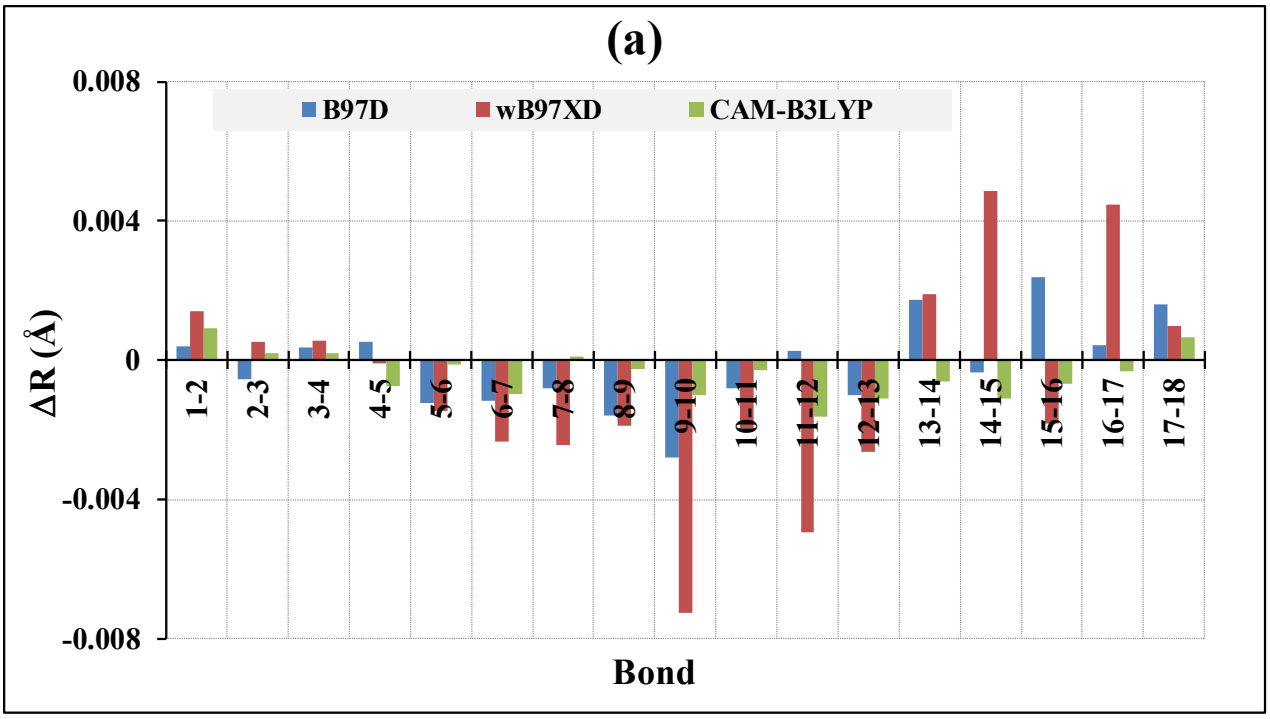
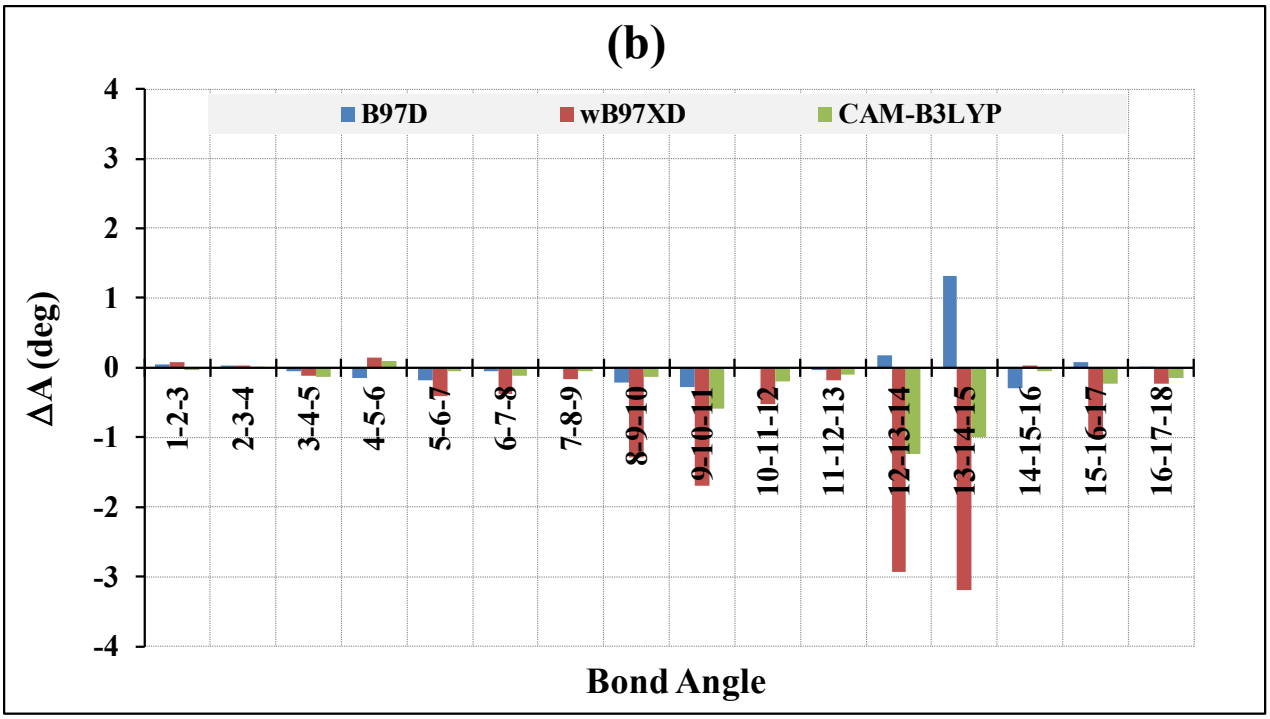


Figure S24. Dispersion effect on geometrical parameters of the DPF-ALD with 2 SCs obtained using B97D, wB97XD, and CAM-B3LYP methods with 6-31G(d) basis set. This figure shows the effect on (a) bond lengths, (b) bond angles, and (c) dihedral angles. The labeling of atoms is shown in Figure 1.


(a)
B97D
wB97XD
CAM-B3LYP
0.008
0.004
0
-0.004
-0.008
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
4
3
2
1
0
-1
-2
-3
-4
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

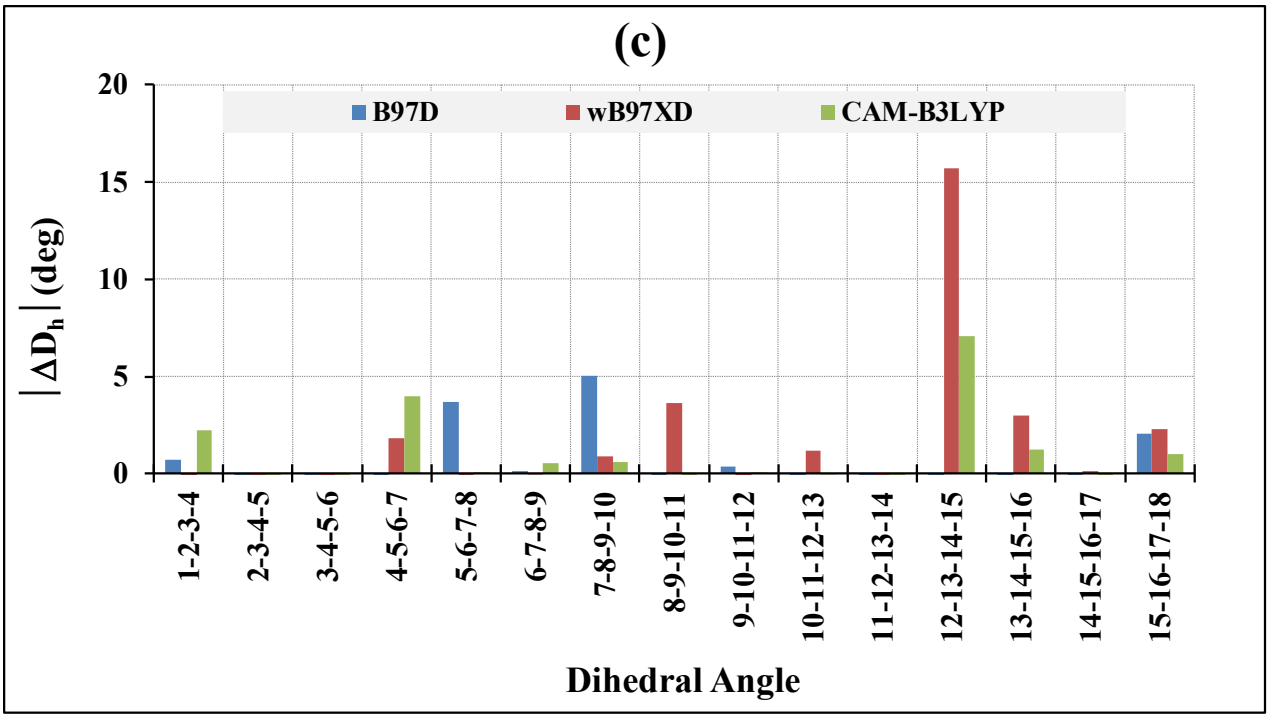
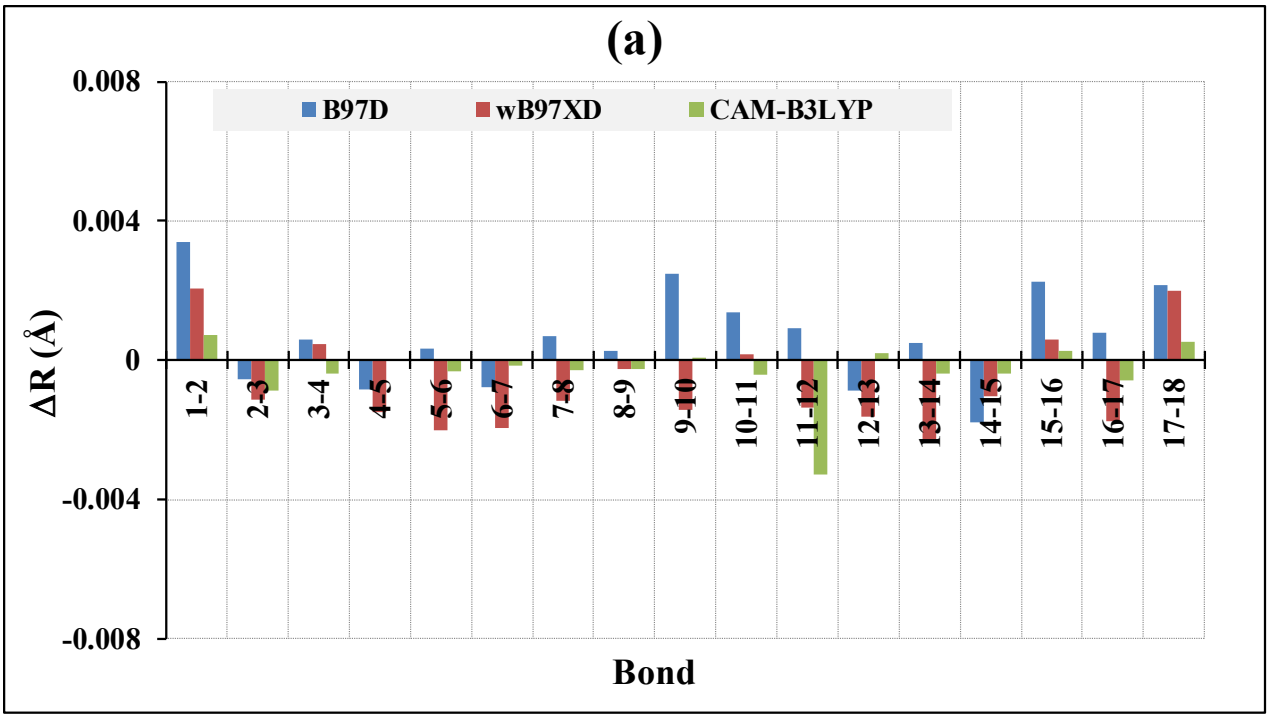
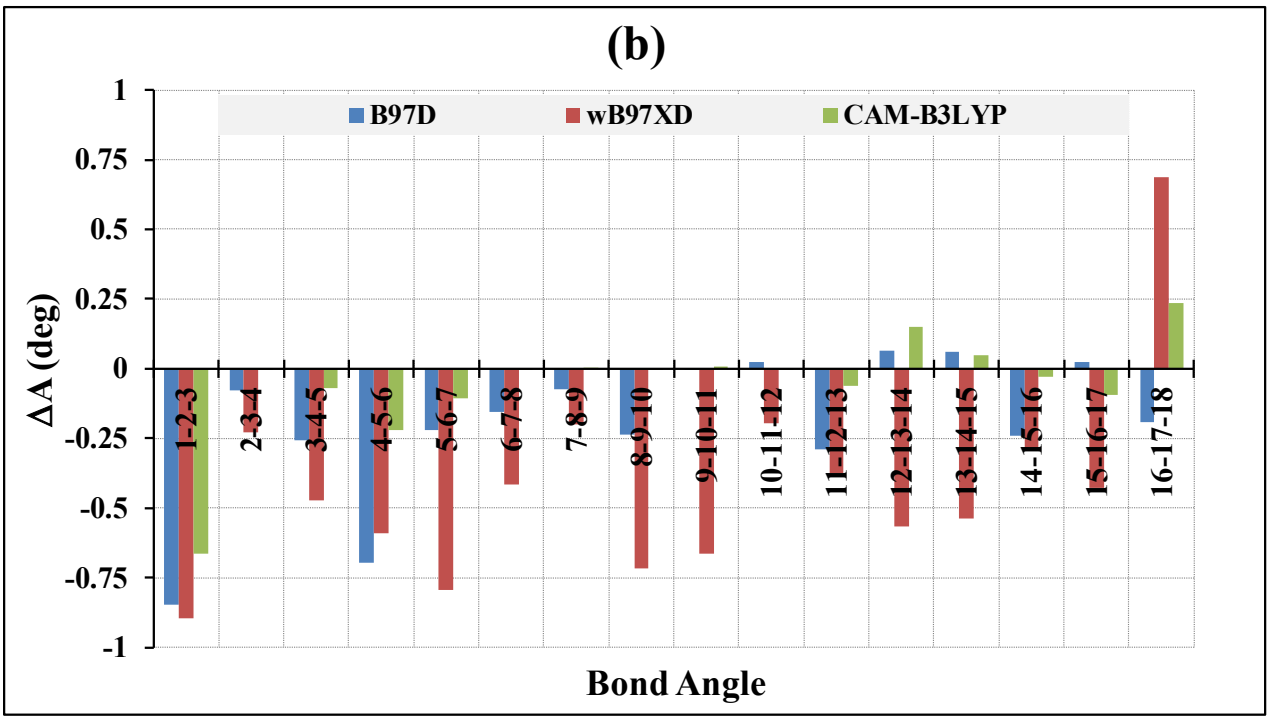


Figure S25. Dispersion effect on geometrical parameters of the DPF-ALD with 6 SCs obtained using B97D, wB97XD, and CAM-B3LYP methods with 6-31G(d) basis set. This figure shows the effect on (a) bond lengths, (b) bond angles, and (c) dihedral angles. The labeling of atoms is shown in Figure 1.


(a)
B97D
wB97XD
CAM-B3LYP
0.008
0.004
0
-0.004
-0.008
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
1
0.75
0.5
0.25
0
-0.25
-0.5
-0.75
-1
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

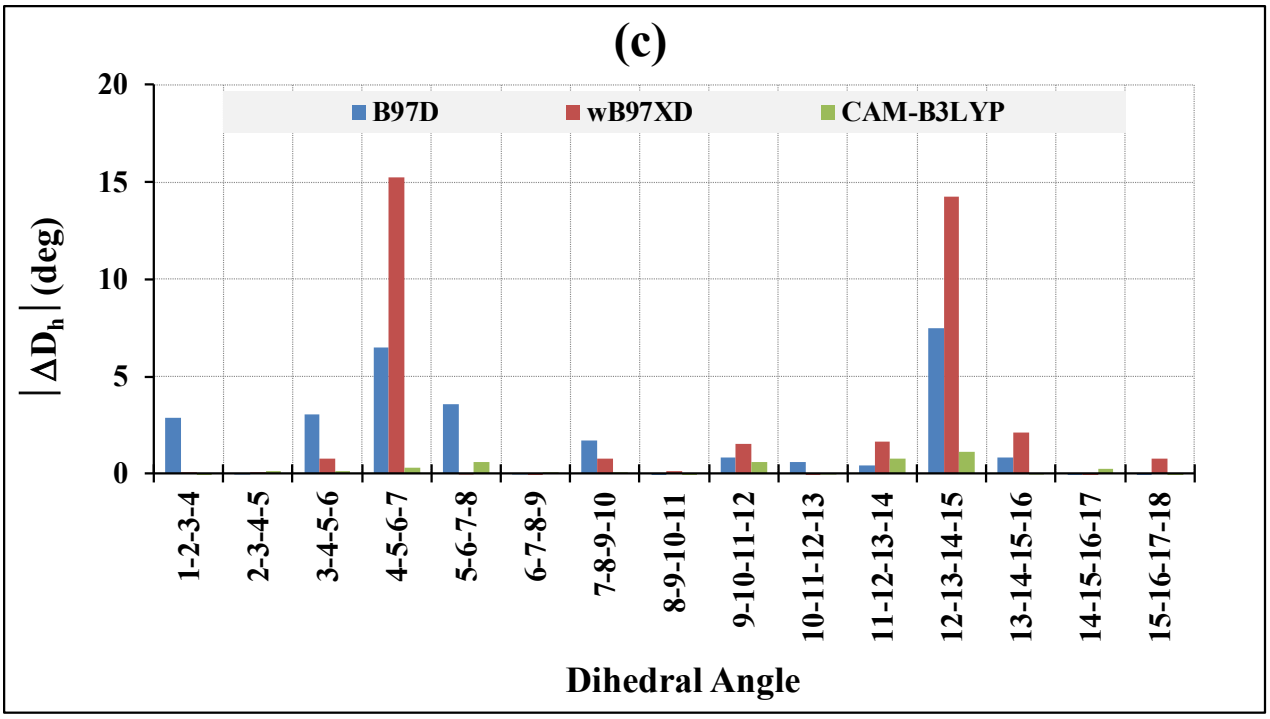
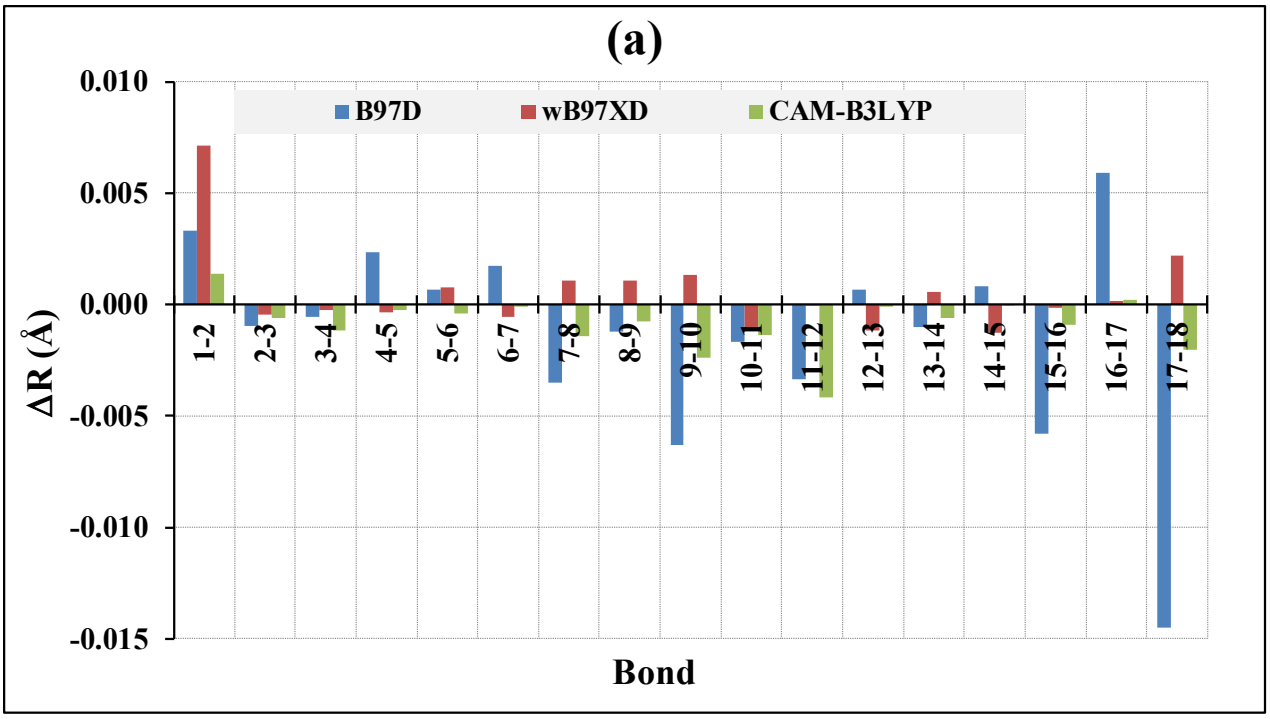
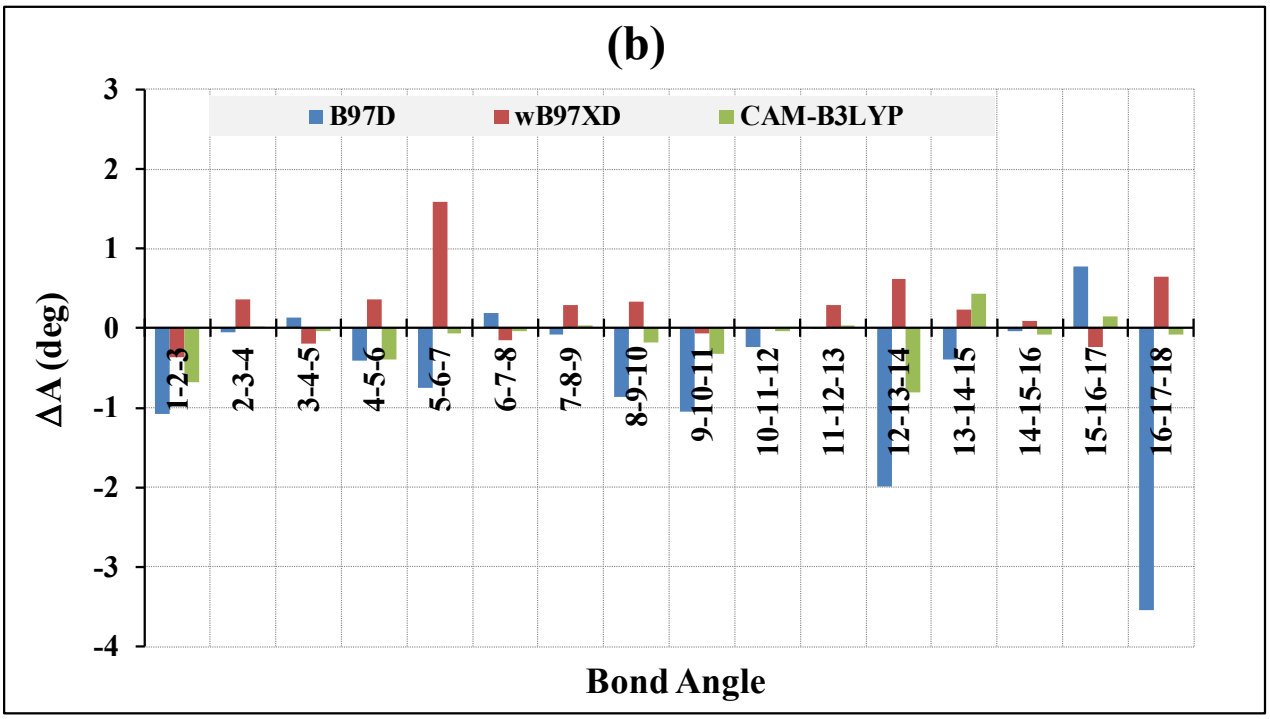


Figure S26. Dispersion effect on geometrical parameters of the DPF-DTF without SCs obtained using B97D, wB97XD, and CAM-B3LYP methods with 6-31G(d) basis set. This figure shows the effect on (a) bond lengths, (b) bond angles, and (c) dihedral angles. The labeling of atoms is shown in Figure 1.


(a)
B97D
wB97XD
CAM-B3LYP
0.010
0.005
0.000
-0.005
-0.010
-0.015
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
3
2
1
0
-1
-2
-3
-4
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

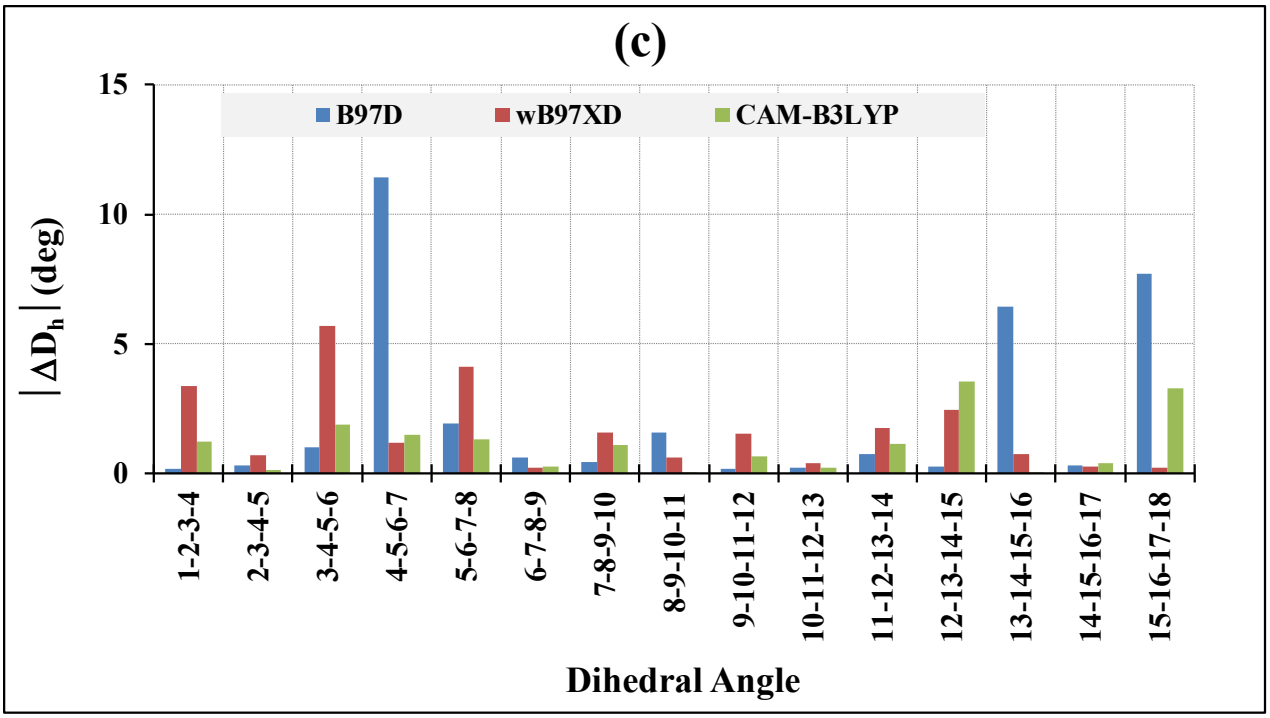
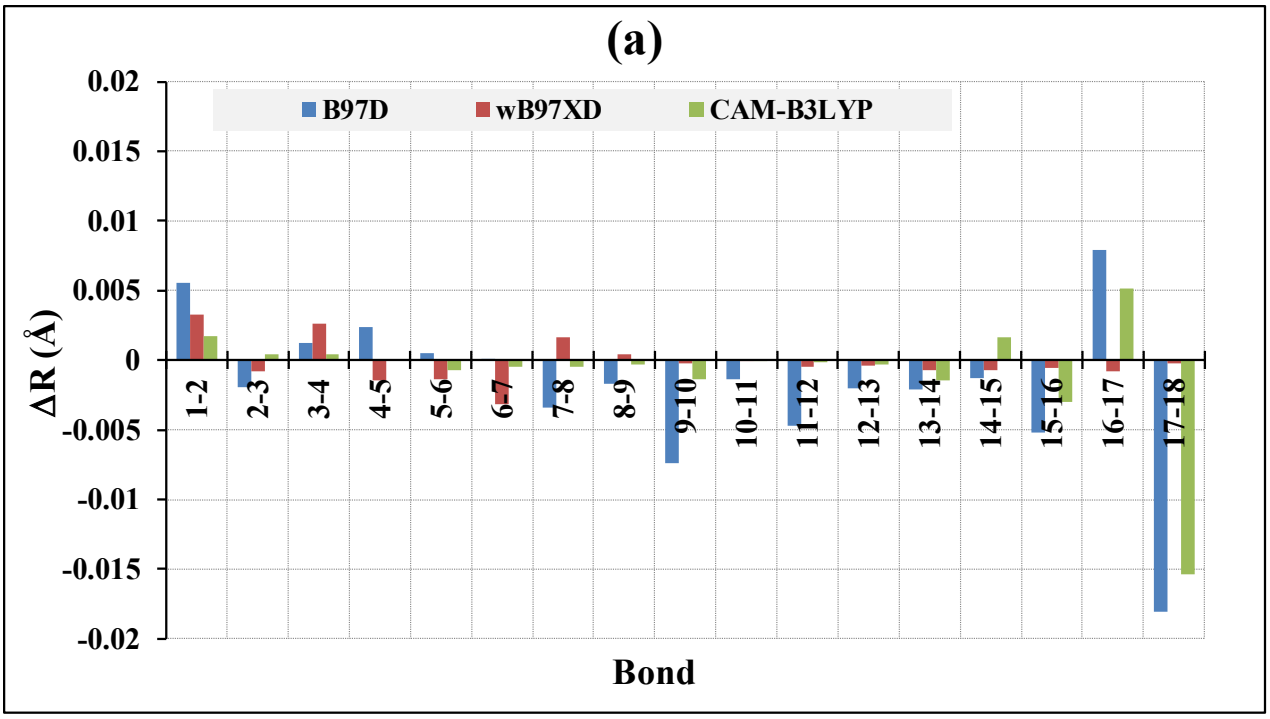
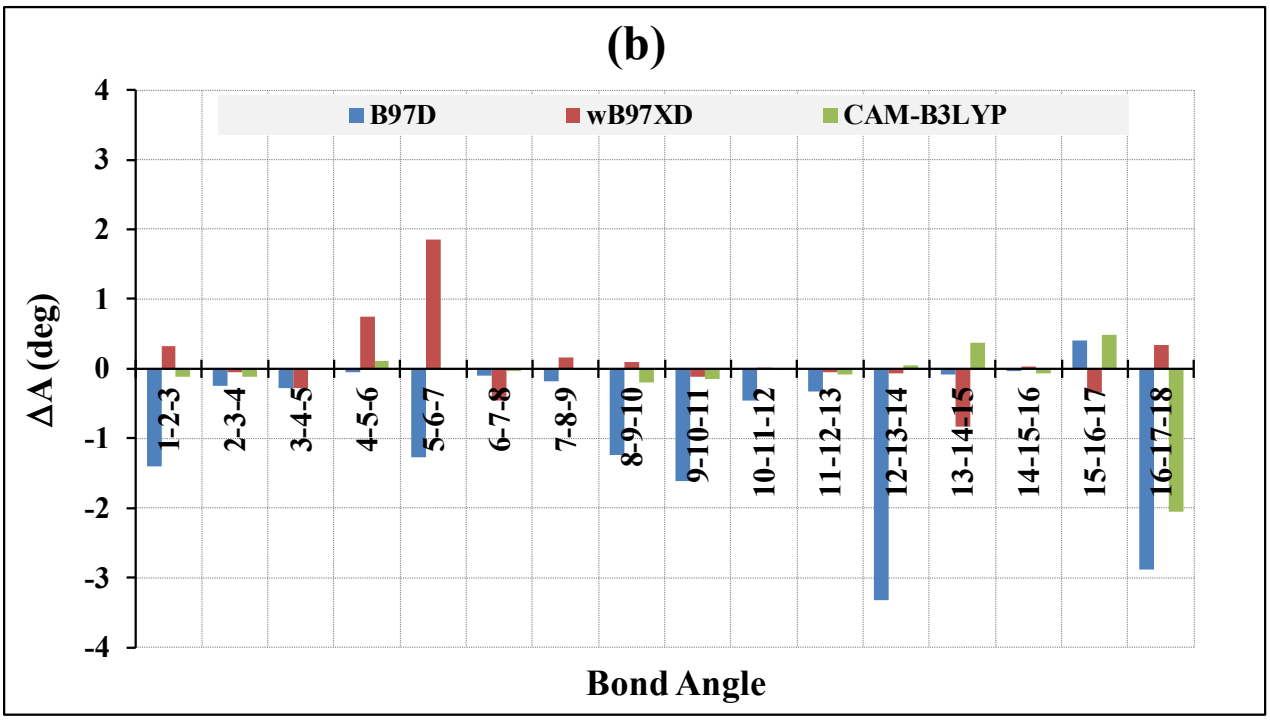


Figure S27. Dispersion effect on geometrical parameters of the DPF-DTF with 6 SCs obtained using B97D, wB97XD, and CAM-B3LYP methods with 6-31G(d) basis set. This figure shows the effect on (a) bond lengths, (b) bond angles, and (c) dihedral angles. The labeling of atoms is shown in Figure 1.


(a)
B97D
wB97XD
CAM-B3LYP
0.02
0.015
0.01
0.005
0
-0.005
-0.01
-0.015
-0.02
ΔR (Å)
1-2
2-3
3-4
4-5
5-6
6-7
7-8
8-9
9-10
10-11
11-12
12-13
13-14
14-15
15-16
16-17
17-18
Bond


(b)
B97D
wB97XD
CAM-B3LYP
4
3
2
1
0
-1
-2
-3
-4
ΔA (deg)
1-2-3
2-3-4
3-4-5
4-5-6
5-6-7
6-7-8
7-8-9
8-9-10
9-10-11
10-11-12
11-12-13
12-13-14
13-14-15
14-15-16
15-16-17
16-17-18
Bond Angle

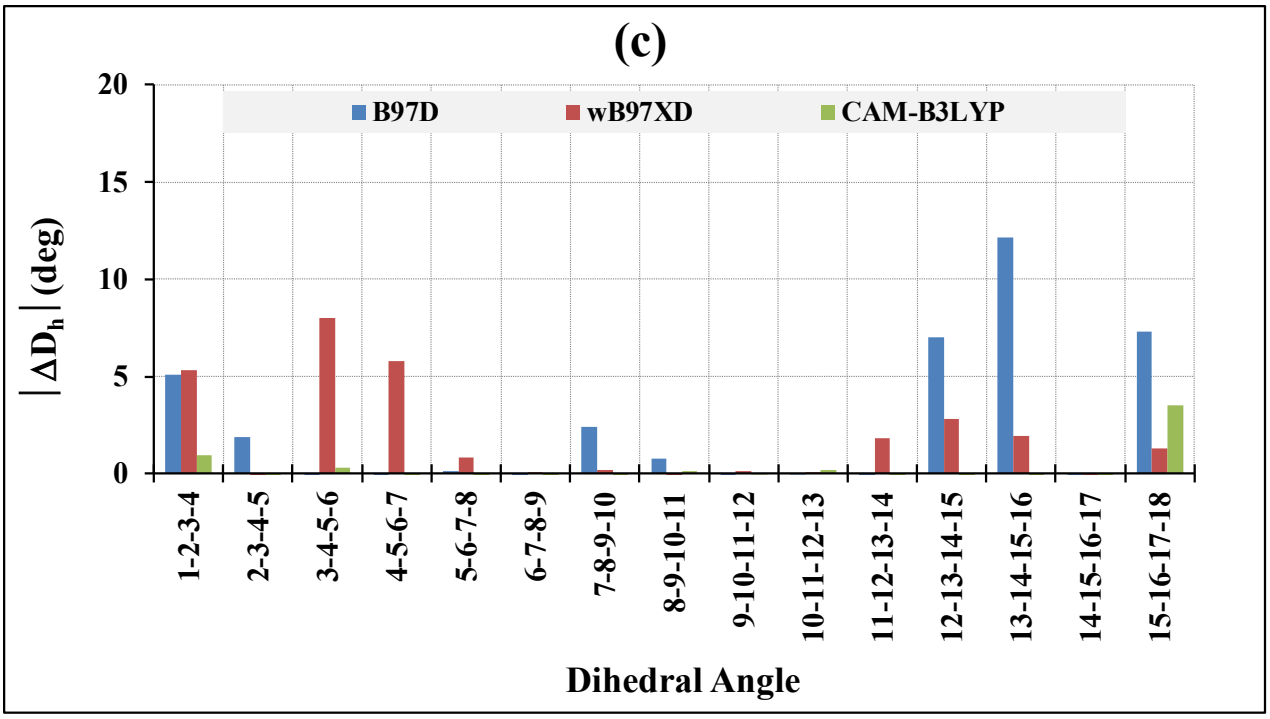


Figure S28. Dispersion effect on geometrical parameters of the DPF-DTF with 10 SCs obtained using B97D, wB97XD, and CAM-B3LYP methods with 6-31G(d) basis set. This figure shows the effect on (a) bond lengths, (b) bond angles, and (c) dihedral angles. The labeling of atoms is shown in Figure 1.