Supporting Information

Interaction of Graphene Quantum Dots with Oligothiophene: A Comprehensive Theoretical Study

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Table of Contents

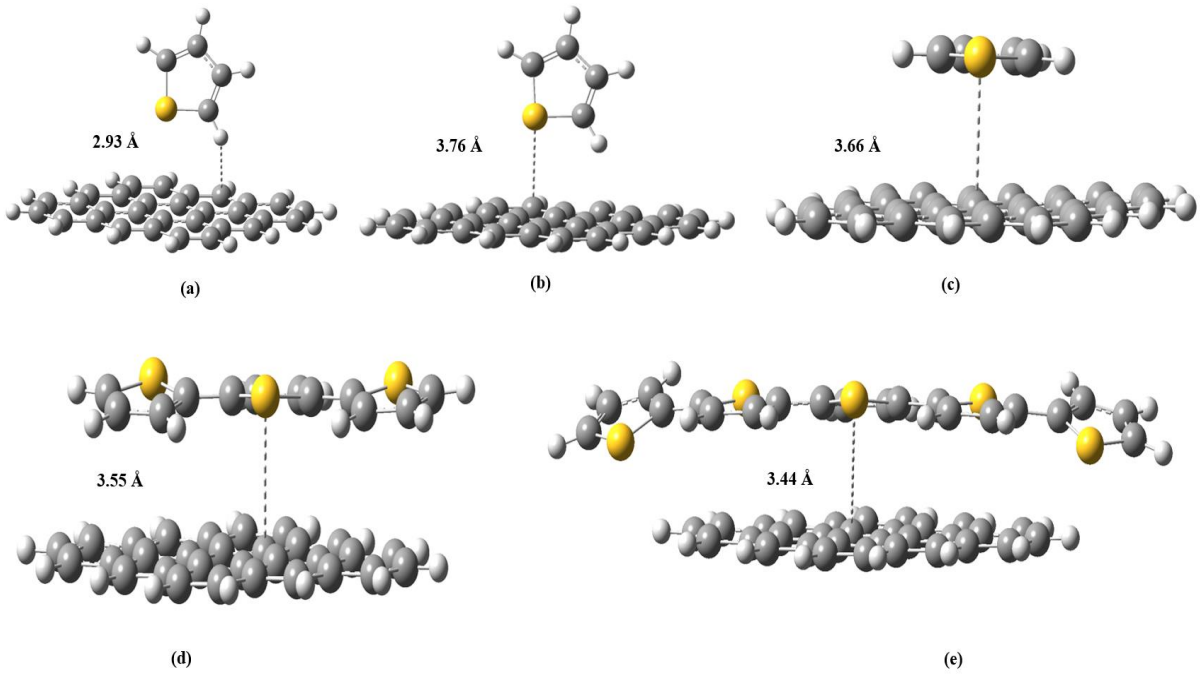

Figure S1: Optimized geometries of (a) vertical CH… π, (b) vertical S... π, (c) stacked $C_{30}H_{14}$ ... 1PT, (d) $C_{30}H_{14}$ ... 3PT and (e) $C_{30}H_{14}$ ... 5PT composites.

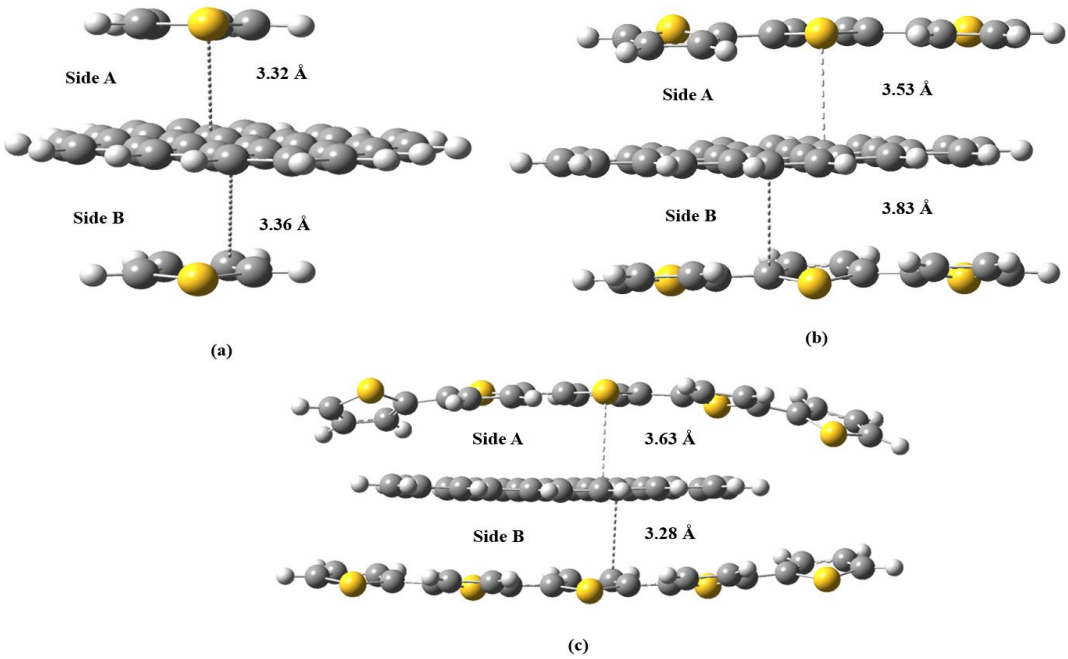

Figure S2: Optimized geometries of (a) stacked 1PT… $C_{30}H_{14}$ … 1PT, (b) 3PT… $C_{30}H_{14}$ … 3PT and (c) 5PT… $C_{30}H_{14}$ … 5PT composites.

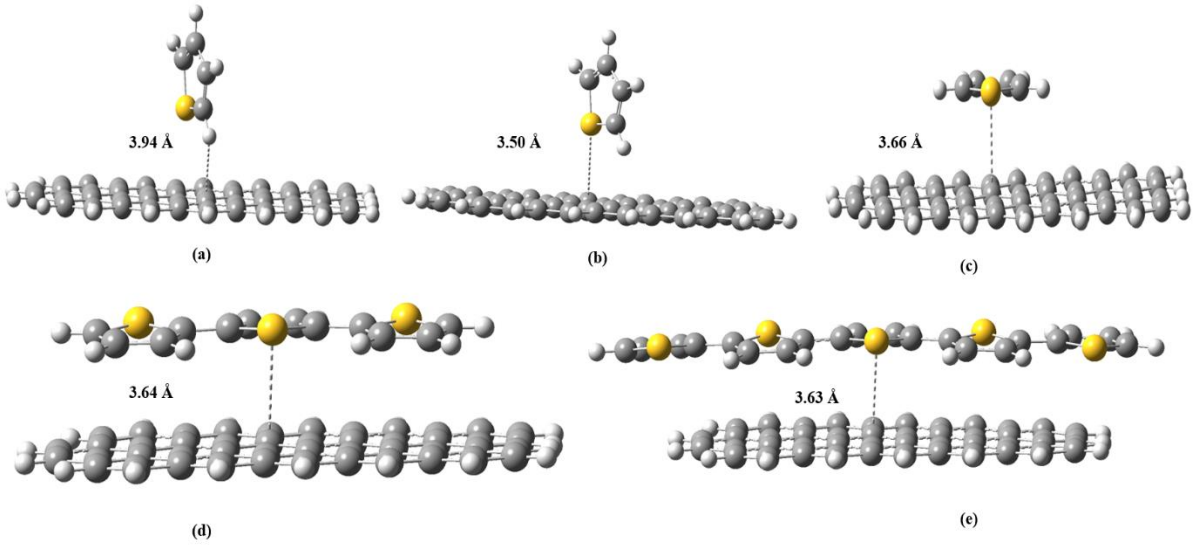

Figure S3: Optimized geometries of (a) vertical CH… π, (b) vertical S... π, (c) stacked $C_{46}H_{18}$ … 1PT, (d) $C_{46}H_{18}$ … 3PT and (e) $C_{46}H_{18}$… 5PT composites.

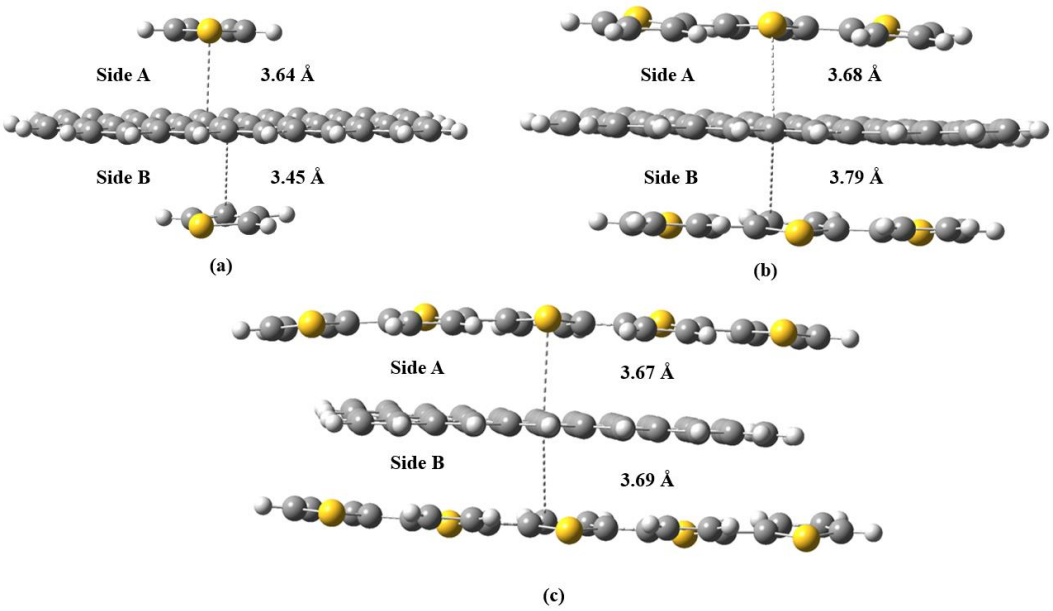

Figure S4: Optimized geometries of (a) stacked 1PT… $C_{46}H_{18}$ … 1PT, (b) 3PT… $C_{46}H_{18}$ … 3PT and (c) 5PT… $C_{46}H_{18}$ … 5PT composites.

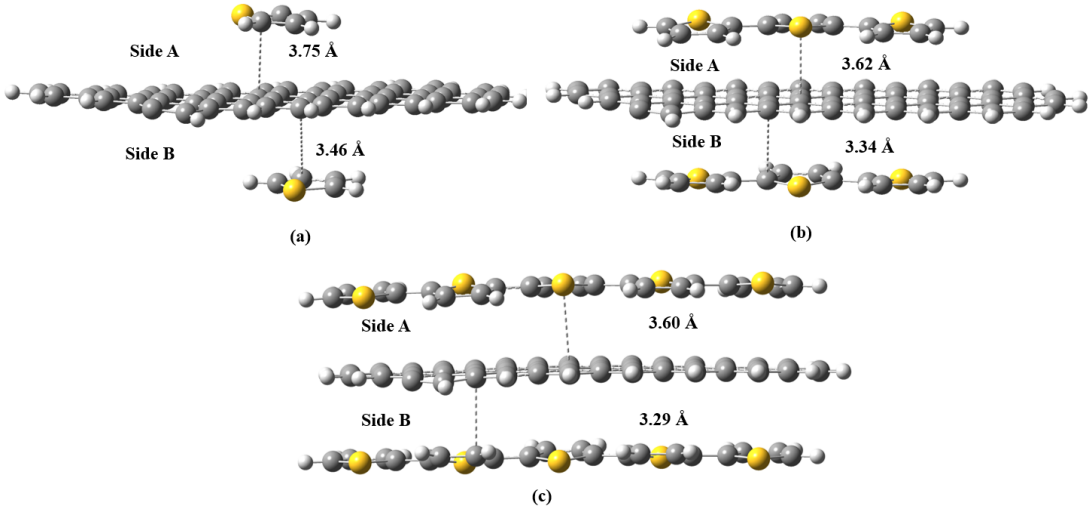

Figure S5: Optimized geometries of (a) stacked 1PT… $C_{59}H_{20}$ … 1PT, (b) 3PT… $C_{59}H_{20}$ … 3PT and (c) 5PT… $C_{59}H_{20}$ … 5PT composites.

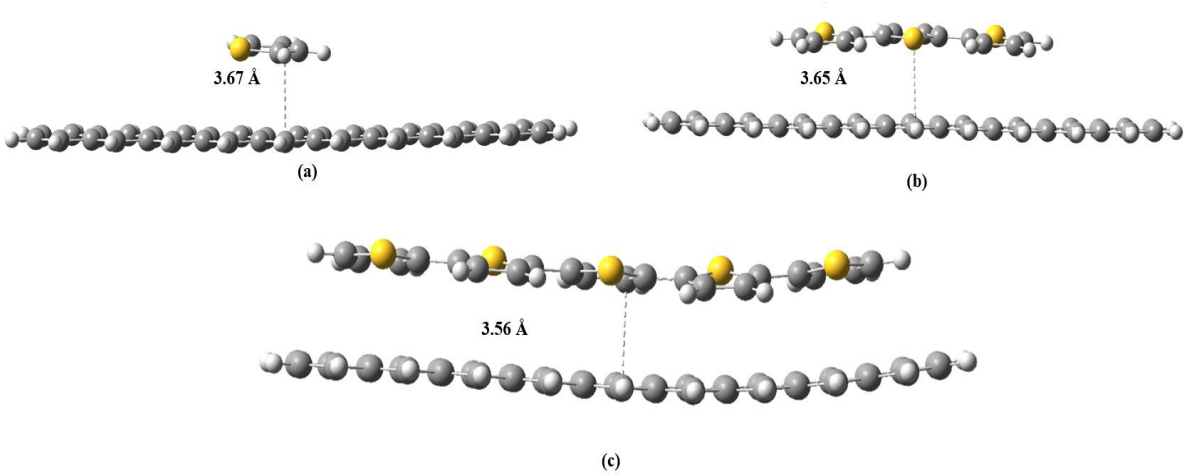

Figure S6: Optimized geometries of (a) stacked $C_{38}H_{22}$ … 1PT, (b) $C_{38}H_{22}$ … 3PT and (c) $C_{38}H_{22}$ … 5PT composites.

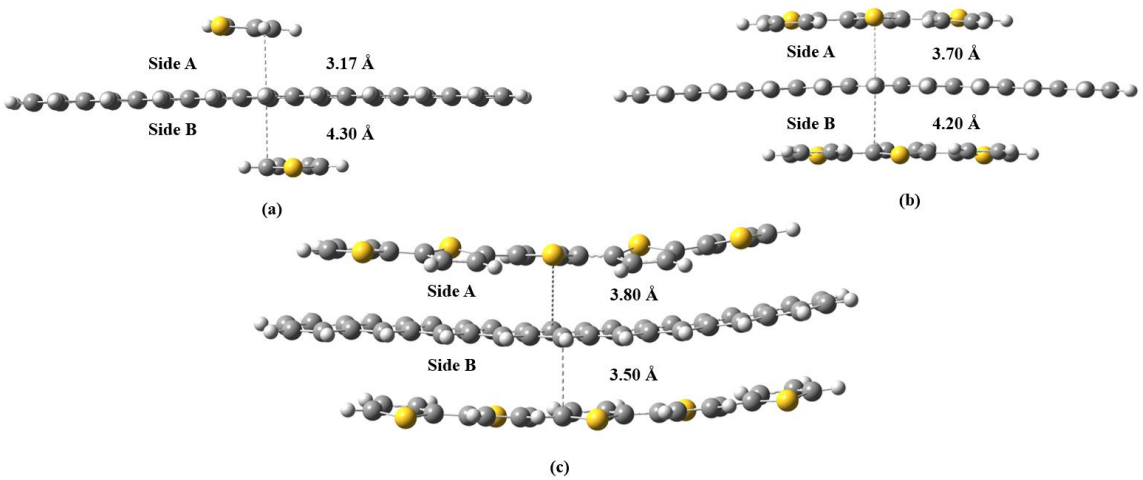

Figure S7: Optimized geometries of (a) stacked 1PT… $C_{38}H_{22}$ … 1PT, (b) 3PT… $C_{38}H_{22}$ … 3PT and (c) 5PT … $C_{38}H_{22}$ … 5PT composites.

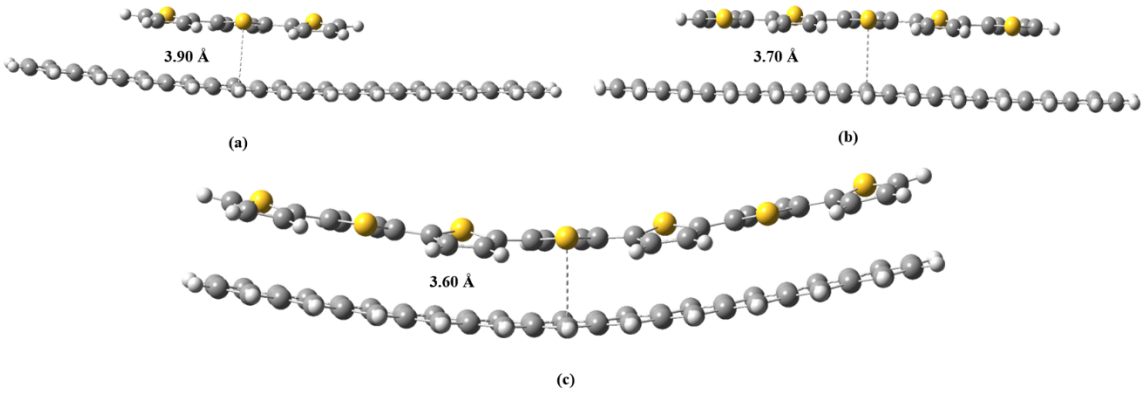

Figure S8: Optimized geometries of (a) stacked $C_{46}H_{26}$ … 3PT, (b) $C_{46}H_{26}$ … 5PT and (c) $C_{46}H_{26}$… 7PT composites.

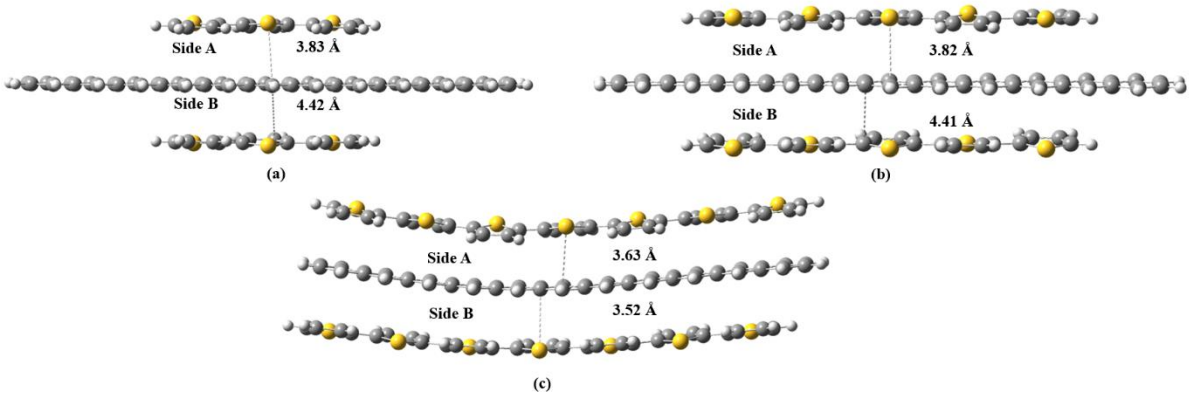

Figure S9: Optimized geometries of (a) stacked 3PT … $C_{46}H_{26}$ … 3PT, (b) 5PT… $C_{46}H_{26}$ … 5PT and (c) 7PT…$C_{46}H_{26}$… 7PT composites.

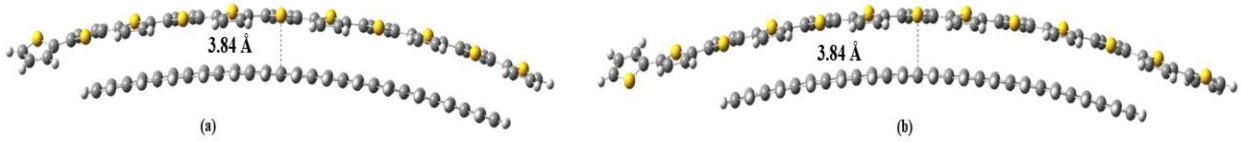

Figure S10: Optimized geometries of (a) stacked $C_{54}H_{30}$ … 11PT and (b) $C_{54}H_{30}$ … 13PT composites

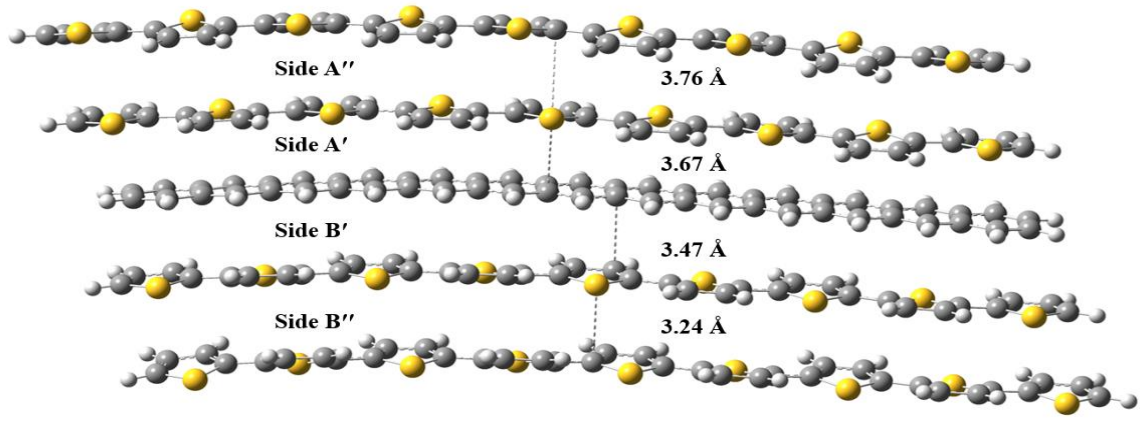

Figure S11: Optimized geometry of 9PT… 9PT… $C_{54}H_{30}$ … 9PT… 9PT composites

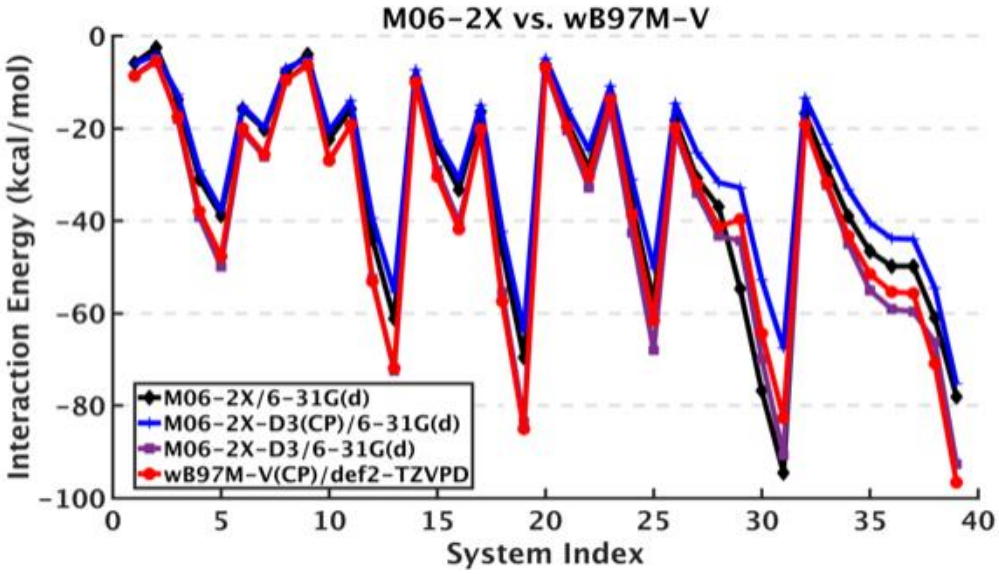

Figure S12: Basis Set comparison with different methods for interaction energy

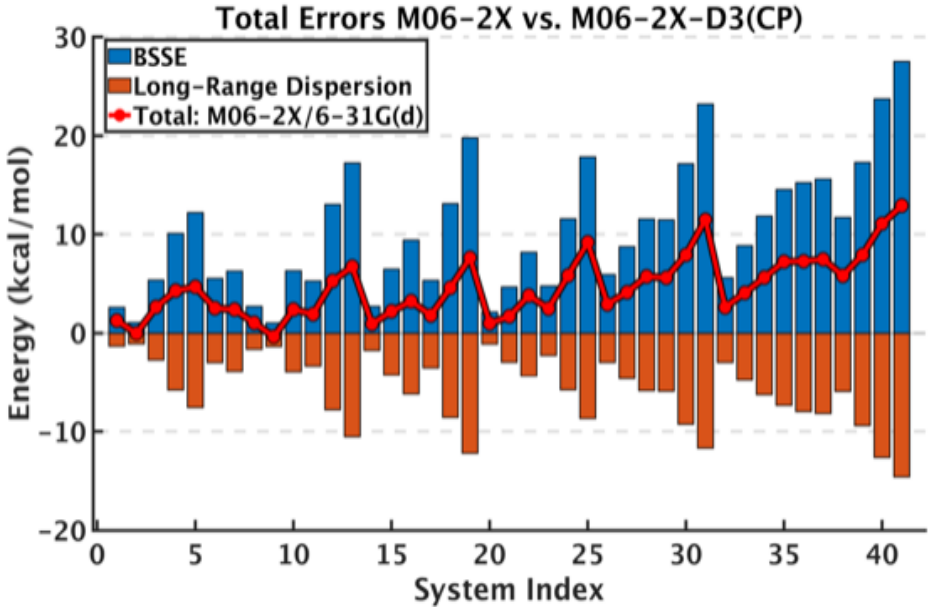

Figure S13: Basis set superposition error (BSSE) and long-range dispersion (D3) error

Table S1: D3 correction values of the interaction energies from M06-2x-D3/6-31G (d) method

System	D3	System	D3
$C_{30}H_{14}$...1PT (stacked)	-1.34	$C_{38}H_{22}$...1PT	-1.13
$C_{30}H_{14}$...1PT (T-shaped)	-1.10	$C_{38}H_{22}$...3PT	-2.97
$C_{30}H_{14}$...3PT	-3.00	$C_{38}H_{22}$...5PT	-4.38
$C_{30}H_{14}$...5PT	-3.89	1PT...$C_{38}H_{22}$...1PT	-2.27
1PT...$C_{30}H_{14}$...1PT	-2.73	3PT...$C_{38}H_{22}$...3PT	-5.79
3PT...$C_{30}H_{14}$...3PT	-5.80	5PT...$C_{38}H_{22}$...5PT	-8.69
5PT...$C_{30}H_{14}$...5PT	-7.56	$C_{46}H_{26}$...3PT	-2.99
$C_{46}H_{18}$...1PT (stacked)	-1.66	$C_{46}H_{26}$...5PT	-4.63
$C_{46}H_{18}$...1PT (T-shaped)	-1.38	$C_{46}H_{26}$...7PT	-5.87
$C_{46}H_{18}$...3PT	-3.92	3PT...$C_{46}H_{26}$...3PT	-5.92
$C_{46}H_{18}$...5PT	-4.35	5PT...$C_{46}H_{26}$...5PT	-9.27
1PT...$C_{46}H_{18}$...1PT	-3.35	7PT...$C_{46}H_{26}$...7PT	-11.69
3PT...$C_{46}H_{18}$...3PT	-7.80	$C_{54}H_{30}$...3PT	-2.99
5PT...$C_{46}H_{18}$...5PT	-10.53	$C_{54}H_{30}$...5PT	-4.78
$C_{59}H_{20}$...1PT (stacked)	-1.76	$C_{54}H_{30}$...7PT	-6.28
$C_{59}H_{20}$...1PT (T-shaped)	-1.45	$C_{54}H_{30}$...9PT	-7.35
$C_{59}H_{20}$...3PT	-4.26	$C_{54}H_{30}$...11PT	-7.98
$C_{59}H_{20}$...5PT	-6.19	$C_{54}H_{30}$...13PT	-8.17
1PT...$C_{59}H_{20}$...1PT	-3.53	3PT...$C_{54}H_{30}$...3PT	-5.94
3PT...$C_{59}H_{20}$...3PT	-8.56	5PT...$C_{54}H_{30}$...5PT	-9.41
5PT...$C_{59}H_{20}$...5PT	-12.20	7PT...$C_{54}H_{30}$...7PT	-12.62
-	-	9PT...$C_{54}H_{30}$...9PT	-14.59

Table S2: Geometric parameters of oligothiophene and graphene nanosheet ($C_{30}H_{14}$…nPT), ($C_{46}H_{18}$ … nPT), ($C_{59}H_{20}$ …nPT) and nano-ribbon ($C_{38}H_{22}$…nPT), ($C_{46}H_{26}$ … nPT), ($C_{54}H_{30}$ …nPT) models

System	Distance Å	System	Interlayer Distance (Å) Side A	Side B
$C_{30}H_{14}$…1PT T-shaped (CH-π)	2.93	-		-
$C_{30}H_{14}$…1PT T-shaped (S-π)	3.76	-		-
$C_{30}H_{14}$…1PT (stacked)	3.66	1PT… $C_{30}H_{14}$…1PT	3.32	3.36
$C_{30}H_{14}$…3PT	3.55	3PT… $C_{30}H_{14}$…3PT	3.53	3.83
$C_{30}H_{14}$…5PT	3.44	5PT… $C_{30}H_{14}$…5PT	3.63	3.28
$C_{46}H_{18}$…1PT T-shaped (CH-π)	3.94	-		-
$C_{46}H_{18}$…1PT T-shaped (S-π)	3.50	-		-
$C_{46}H_{18}$…1PT (stacked)	3.66	1PT… $C_{46}H_{18}$…1PT	3.64	3.45
$C_{46}H_{18}$…3PT	3.64	3PT… $C_{46}H_{18}$…3PT	3.68	3.79
$C_{46}H_{18}$…5PT	3.63	5PT… $C_{46}H_{18}$…5PT	3.67	3.69
$C_{59}H_{20}$…1PT T-shaped (CH-π)	3.49	-		-
$C_{59}H_{20}$…1PT T-shaped (S-π)	3.64	-		-
$C_{59}H_{20}$…1PT (stacked)	3.62	1PT… $C_{59}H_{20}$…1PT	3.75	3.46
$C_{59}H_{20}$…3PT	3.65	3PT… $C_{59}H_{20}$…3PT	3.62	3.34
$C_{59}H_{20}$…5PT	3.55	5PT… $C_{59}H_{20}$…5PT	3.60	3.29
$C_{38}H_{22}$…1PT	3.67	1PT… $C_{38}H_{22}$…1PT	3.17	4.30
$C_{38}H_{22}$…3PT	3.65	3PT… $C_{38}H_{22}$…3PT	3.70	4.20
$C_{38}H_{22}$…5PT	3.56	5PT… $C_{38}H_{22}$…5PT	3.80	3.50
$C_{46}H_{26}$…3PT	3.90	3PT… $C_{46}H_{26}$…3PT	3.83	4.42
$C_{46}H_{26}$…5PT	3.70	5PT… $C_{46}H_{26}$…5PT	3.82	4.41
$C_{46}H_{26}$…7PT	3.60	7PT… $C_{46}H_{26}$…7PT	3.63	3.52
$C_{54}H_{30}$…3PT	3.60	3PT… $C_{54}H_{30}$…3PT	3.58	4.74
$C_{54}H_{30}$…5PT	3.96	5PT… $C_{54}H_{30}$…5PT	3.84	4.45
$C_{54}H_{30}$…7PT	3.85	7PT… $C_{54}H_{30}$…7PT	3.83	4.43
$C_{54}H_{30}$…9PT	3.83	9PT… $C_{54}H_{30}$…9PT	3.81	4.41
$C_{54}H_{30}$…11PT	3.84	-	-	-
$C_{54}H_{30}$…13PT	3.84	-	-	-

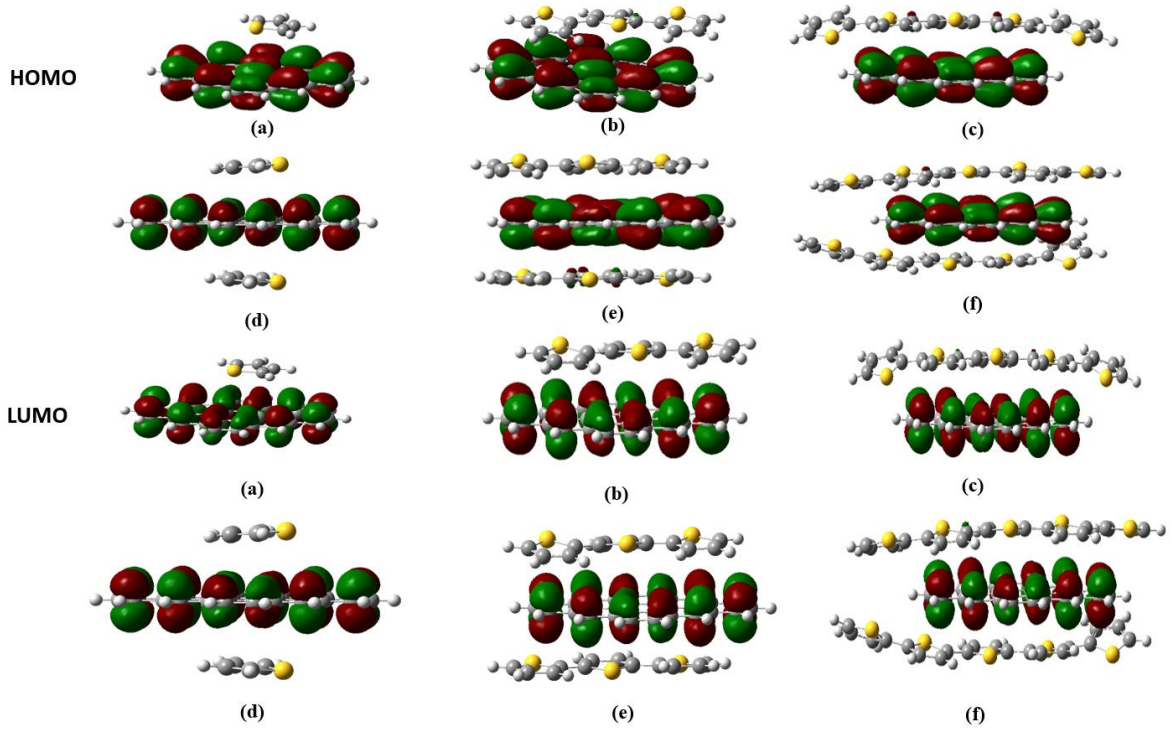

Figure S14: Canonical depiction of HOMO orbitals of (a) $C_{30}H_{14}$ ... 1PT, (b) $C_{30}H_{14}$ ... 3PT, (c) $C_{30}H_{14}$... 5PT, (d) 1PT… $C_{30}H_{14}$ ... 1PT, (e) 3PT… $C_{30}H_{14}$ ... 3PT, (f) 5PT… $C_{30}H_{14}$ ... 5PT and LUMO orbitals of (a) $C_{30}H_{14}$ ... 1PT, (b) $C_{30}H_{14}$ ... 3PT, (c) $C_{30}H_{14}$... 5PT, (d) 1PT… $C_{30}H_{14}$ ... 1PT, (e) 3PT… $C_{30}H_{14}$ ... 3PT, (f) 5PT… $C_{30}H_{14}$ ... 5PT composites

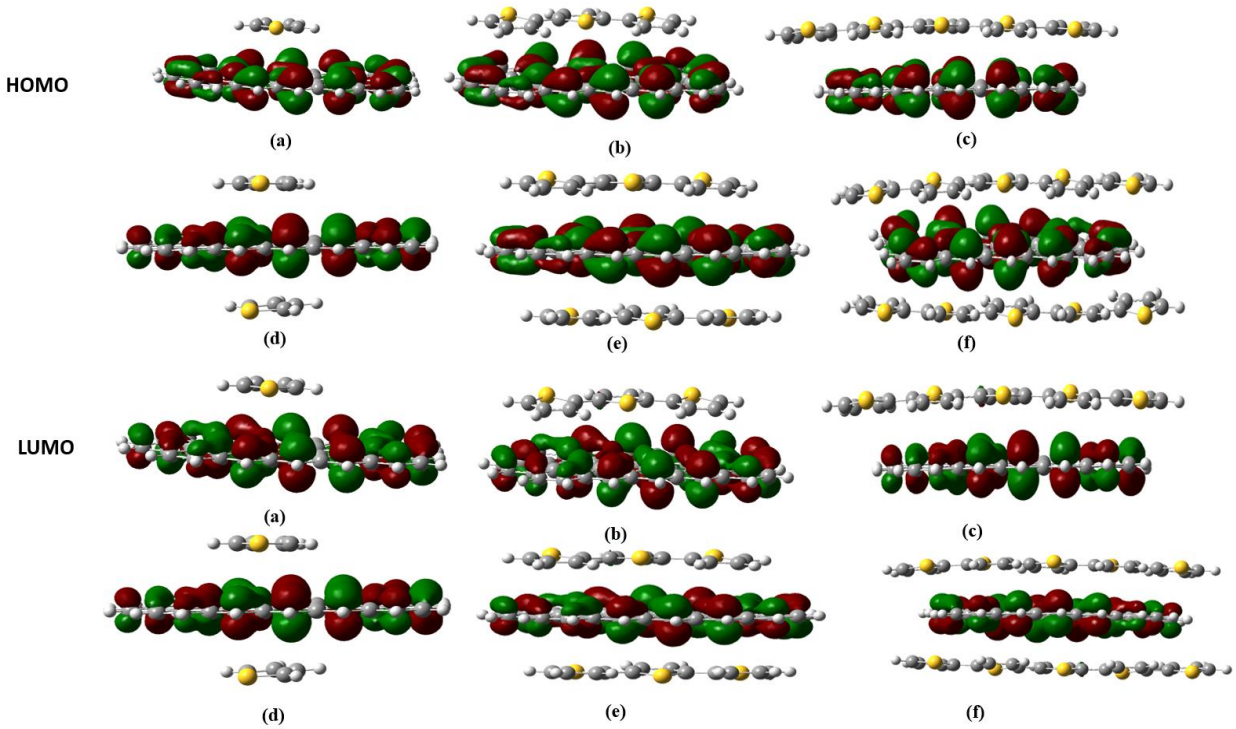

Figure S15: Canonical depiction of HOMO orbitals of (a) $C_{46}H_{18}$ ... 1PT, (b) $C_{46}H_{18}$ ... 3PT, (c) $C_{46}H_{18}$... 5PT, (d) 1PT… $C_{46}H_{18}$ ... 1PT, (e) 3PT… $C_{46}H_{18}$... 3PT, (f) 5PT… $C_{46}H_{18}$ ... 5PT and LUMO orbitals of (a) $C_{46}H_{18}$ ... 1PT, (b) $C_{46}H_{18}$ ... 3PT, (c) $C_{46}H_{18}$... 5PT, (d) 1PT… $C_{46}H_{18}$ ... 1PT, (e) 3PT… $C_{46}H_{18}$ ... 3PT, (f) 5PT… $C_{46}H_{18}$ ... 5PT composites

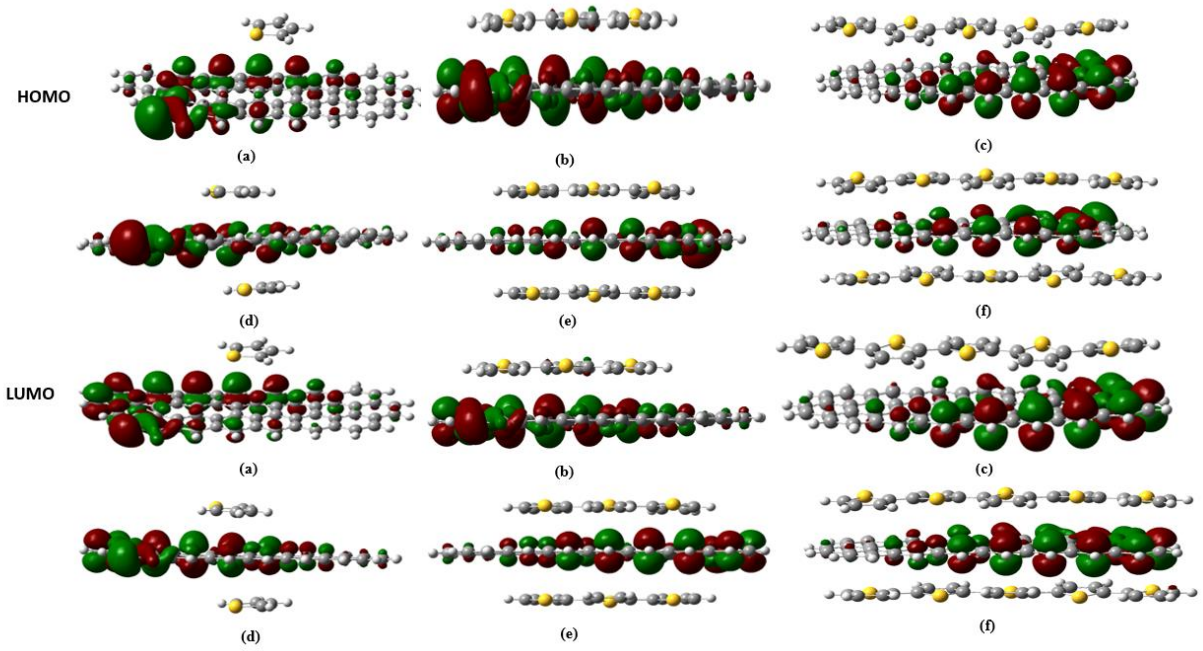

Figure S16: Canonical depiction of HOMO orbitals of (a) $C_{59}H_{20}$ ... 1PT, (b) $C_{59}H_{20}$ ... 3PT, (c) $C_{59}H_{20}$... 5PT, (d) 1PT… $C_{59}H_{20}$ ... 1PT, (e) 3PT… $C_{59}H_{20}$ ... 3PT, (f) 5PT… $C_{59}H_{20}$ ... 5PT and LUMO orbitals of (a) $C_{59}H_{20}$ ... 1PT, (b) $C_{59}H_{20}$ ... 3PT, (c) $C_{59}H_{20}$... 5PT, (d) 1PT… $C_{59}H_{20}$ ... 1PT, (e) 3PT… $C_{59}H_{20}$ ... 3PT, (f) 5PT… $C_{59}H_{20}$ ... 5PT composites

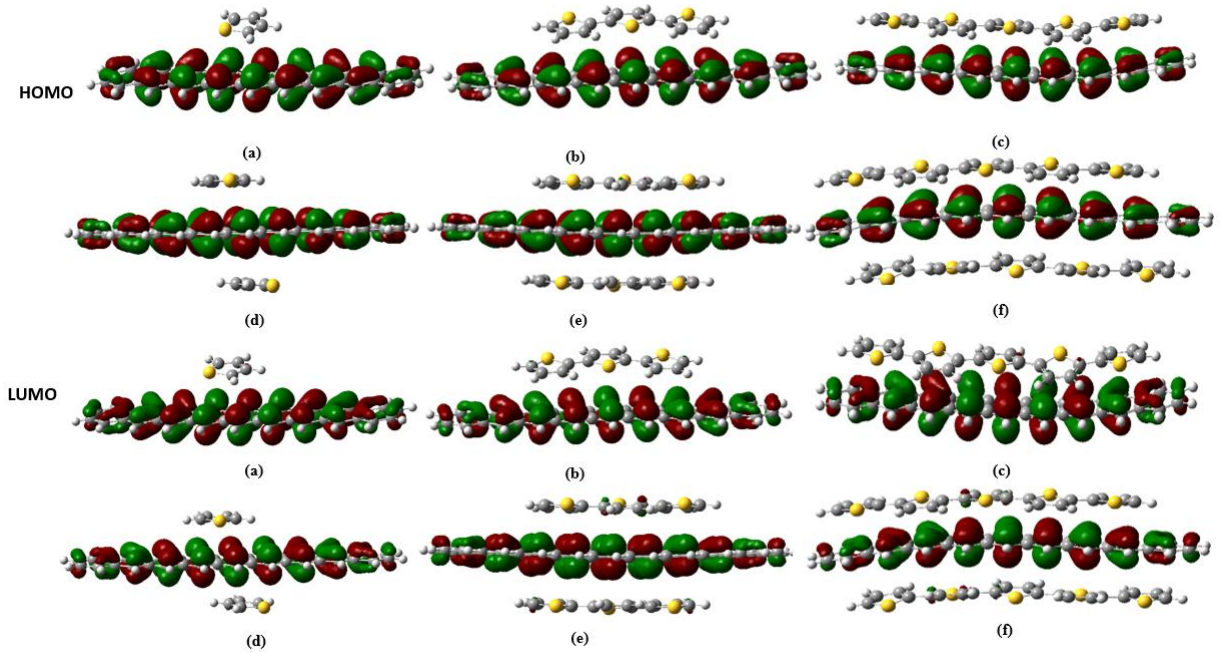

Figure S17: Canonical depiction of HOMO orbitals of (a) $C_{38}H_{22}$ ... 1PT, (b) $C_{38}H_{22}$ ... 3PT, (c) $C_{38}H_{22}$... 5PT, (d) 1PT… $C_{38}H_{22}$ ... 1PT, (e) 3PT… $C_{38}H_{22}$... 3PT, (f) 5PT… $C_{38}H_{22}$ ... 5PT and LUMO orbitals of (a) $C_{38}H_{22}$ ... 1PT, (b) $C_{38}H_{22}$ ... 3PT, (c) $C_{38}H_{22}$... 5PT, (d) 1PT… $C_{38}H_{22}$... 1PT, (e) 3PT… $C_{38}H_{22}$... 3PT, (f) 5PT… $C_{38}H_{22}$... 5PT composites

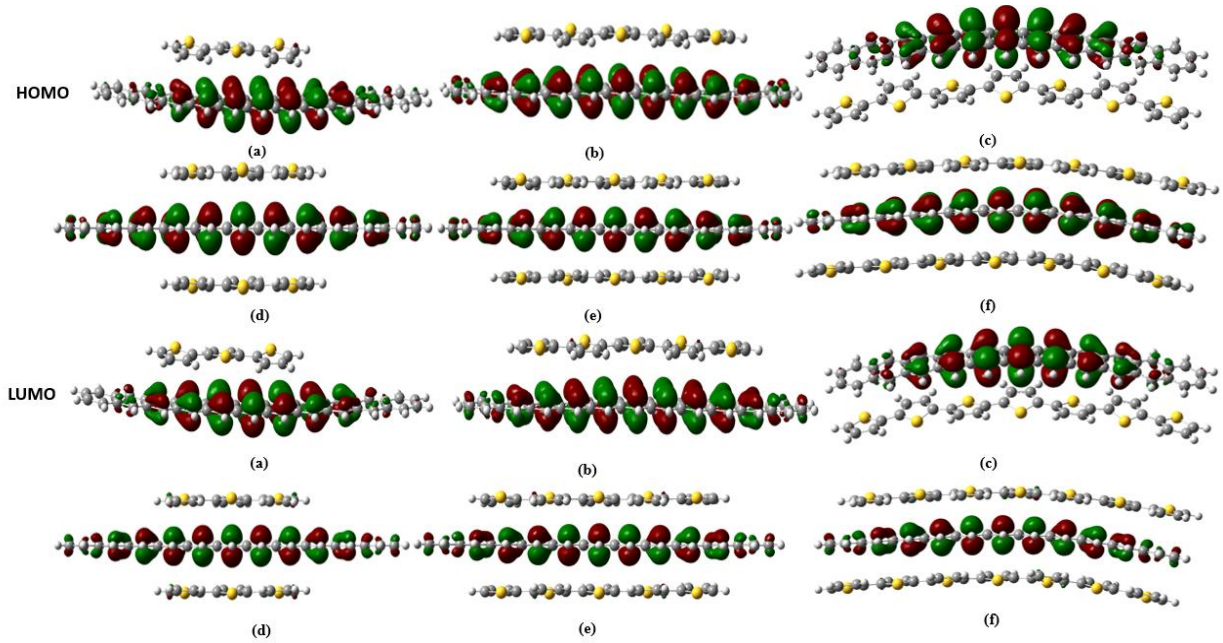

Figure S18: Canonical depiction of HOMO orbitals of (a) $C_{46}H_{26}$ ... 3PT, (b) $C_{46}H_{26}$ ... 5PT, (c) $C_{46}H_{26}$ ... 7PT, (d) 3PT… $C_{46}H_{26}$ ... 3PT, (e) 5PT… $C_{46}H_{26}$ ... 5PT, (f) 7PT… $C_{46}H_{26}$ ... 7PT and LUMO orbitals of (a) $C_{46}H_{26}$ ... 3PT, (b) $C_{46}H_{26}$ ... 5PT, (c) $C_{46}H_{26}$ ... 7PT, (d) 3PT… $C_{46}H_{26}$ ... 3PT, (e) 5PT… $C_{46}H_{26}$ ... 5PT, (f) 7PT… $C_{46}H_{26}$ ... 7PT composites

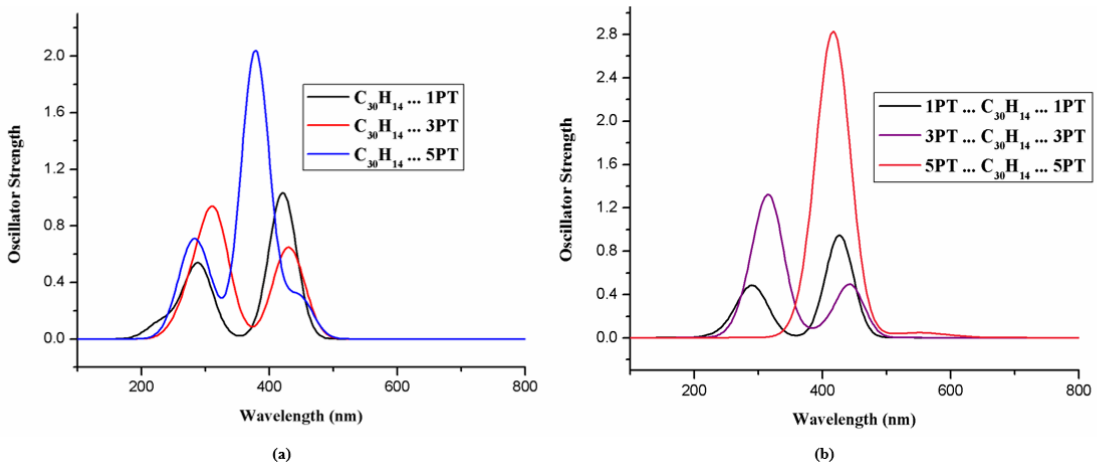

Figure S19: UV-vis spectra of (a) $C_{30}H_{14}$ ... nPT and (b) nPT… $C_{30}H_{14}$... nPT composites

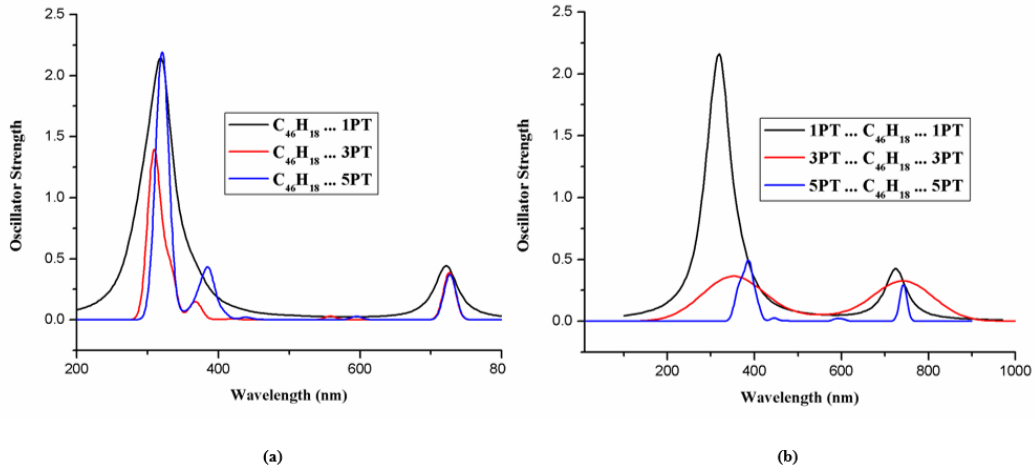

Figure S20: UV-vis spectra of (a) $C_{46}H_{18}$ ... nPT and (b) nPT… $C_{46}H_{18}$... nPT composites

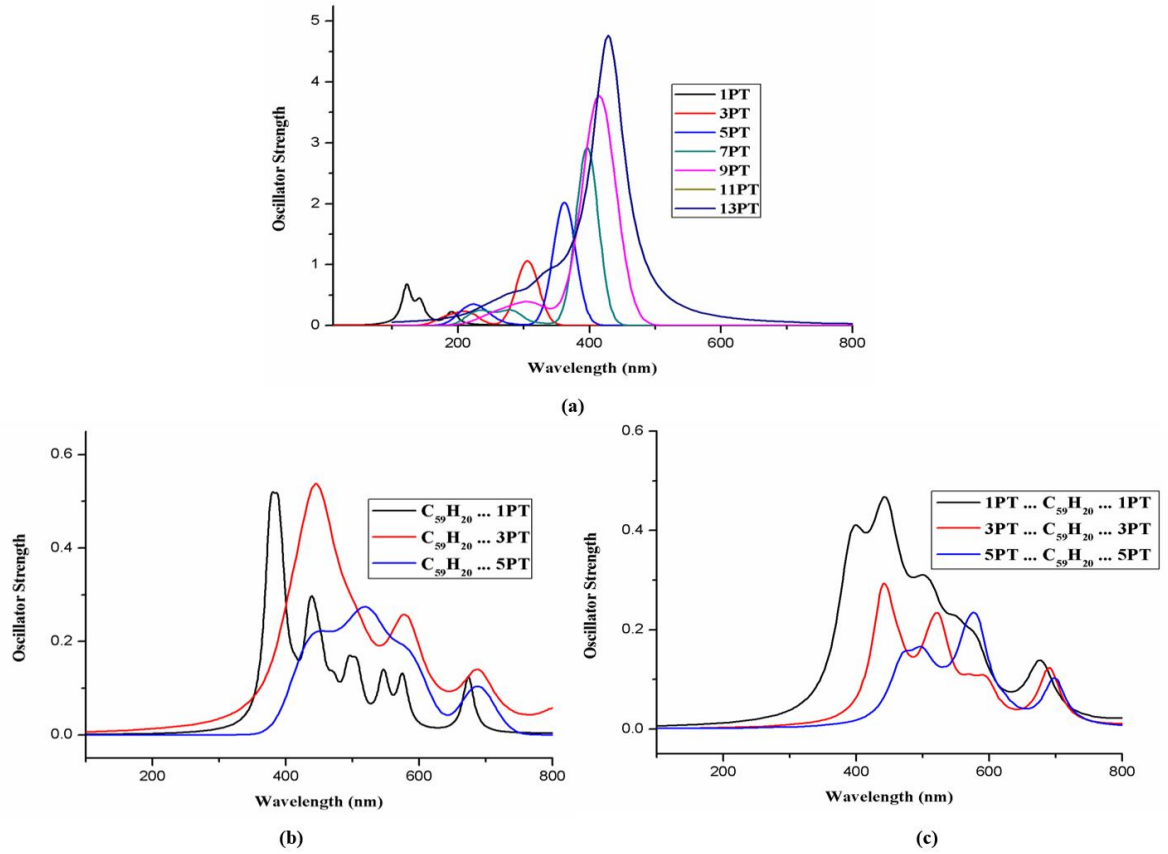

Figure S21: UV-vis spectra of (a) isolated oligothiophene, (b) $C_{59}H_{20}$ ... nPT and (c) nPT… $C_{59}H_{20}$... nPT composites

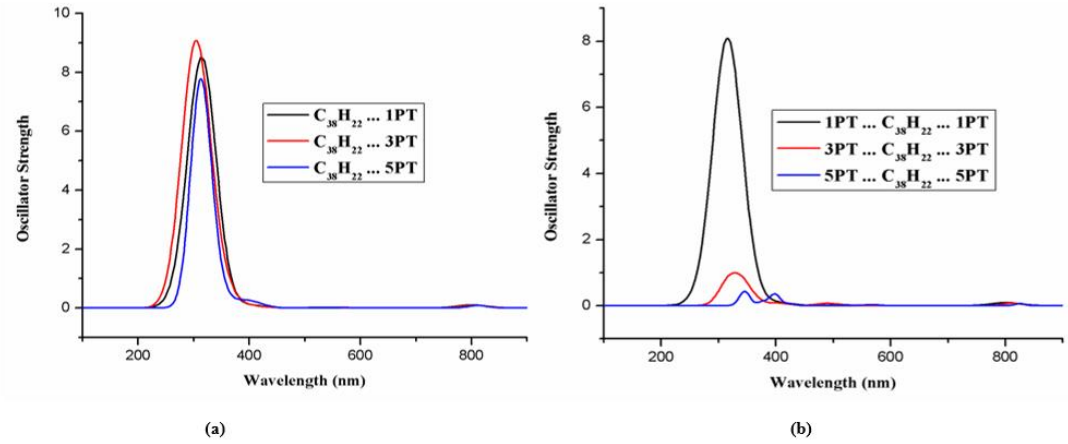

Figure S22: UV-vis spectra of (a) $C_{38}H_{22}$ ... nPT and (b) nPT… $C_{38}H_{22}$... nPT composites

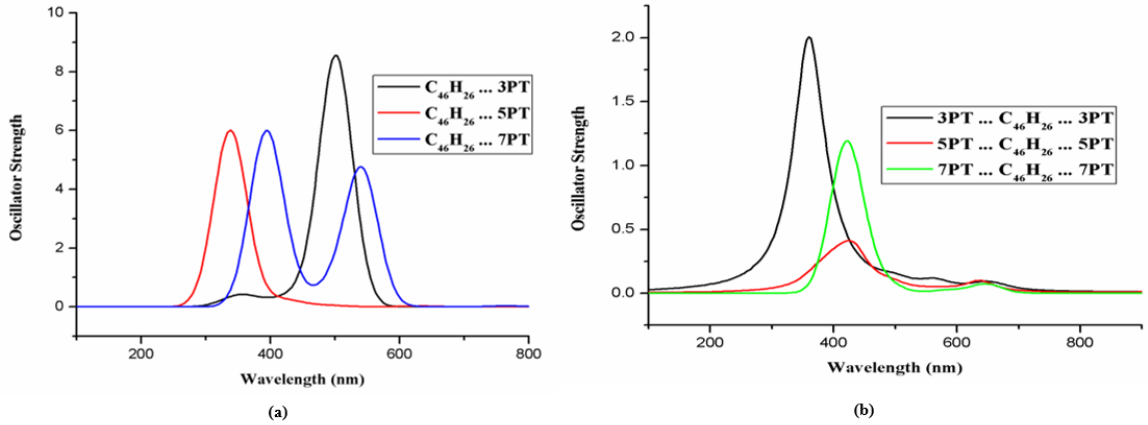

Figure S23: UV-vis spectra of (a) $C_{46}H_{26}$ ... nPT and (b) nPT… $C_{46}H_{26}$... nPT composites

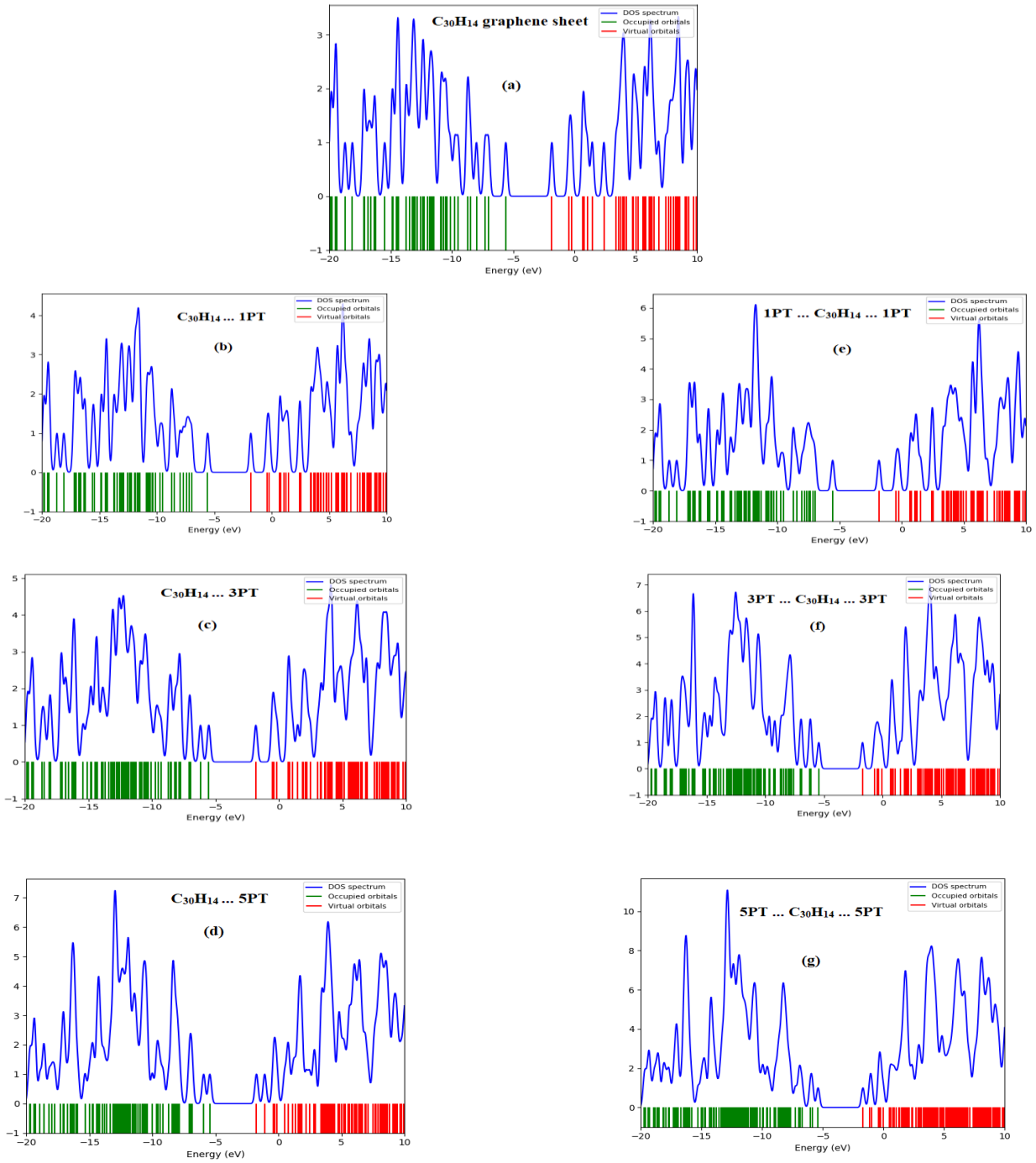

Figure S24: DOS spectra of (a) $C_{30}H_{14}$ (b) $C_{30}H_{14}$ ... 1PT, (c) $C_{30}H_{14}$ ... 3PT, (d) $C_{30}H_{14}$... 5PT, (e) 1PT… $C_{30}H_{14}$ ... 1PT, (f) 3PT… $C_{30}H_{14}$ ... 3PT, (g) 5PT… $C_{30}H_{14}$ ... 5PT composites

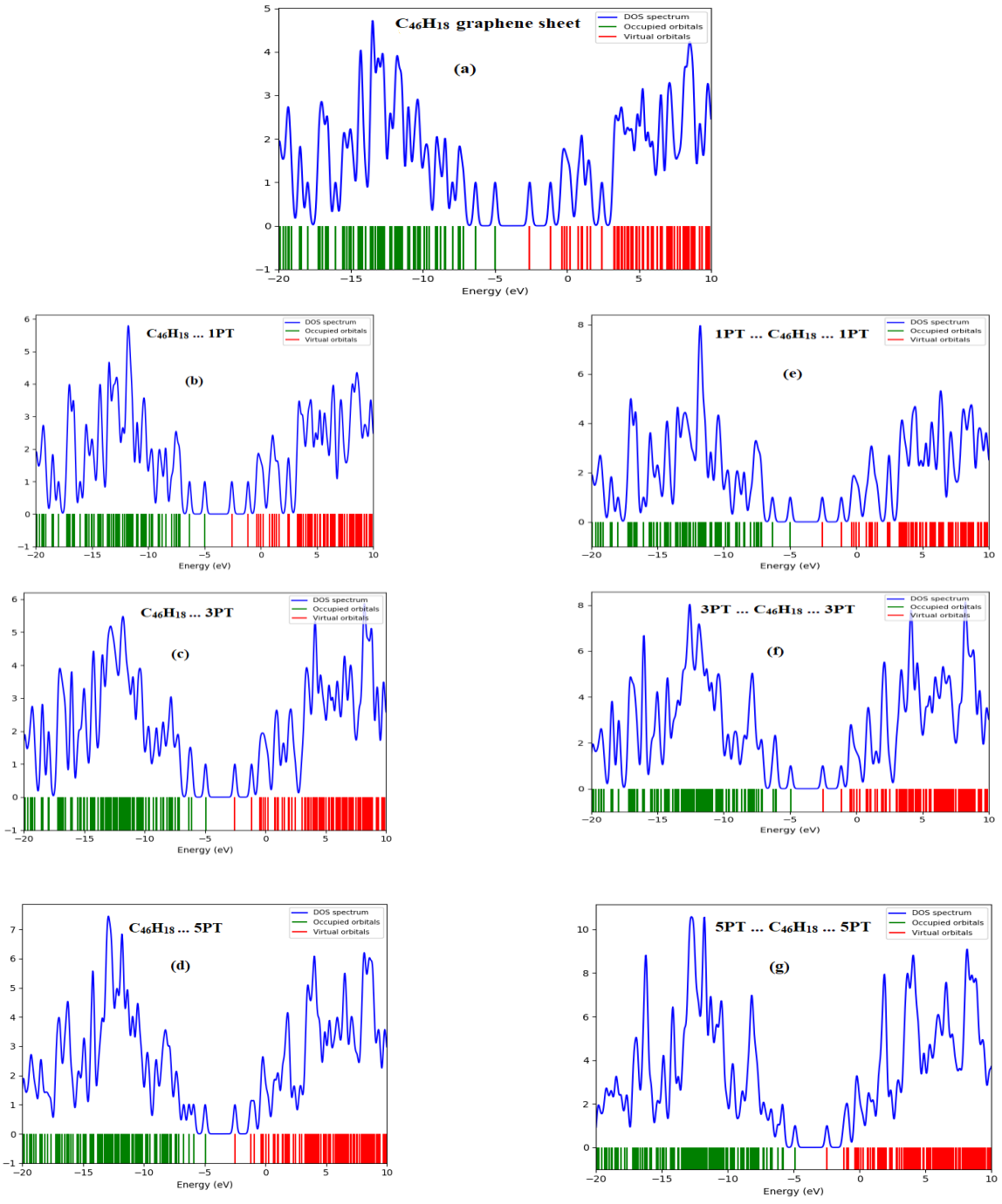

Figure S25: DOS spectra of (a) $C_{46}H_{18}$ (b) $C_{46}H_{18}$ ... 1PT, (c) $C_{46}H_{18}$ ... 3PT, (d) $C_{46}H_{18}$... 5PT, (e) 1PT… $C_{46}H_{18}$ ... 1PT, (f) 3PT… $C_{46}H_{18}$... 3PT, (g) 5PT… $C_{46}H_{18}$ ... 5PT composite

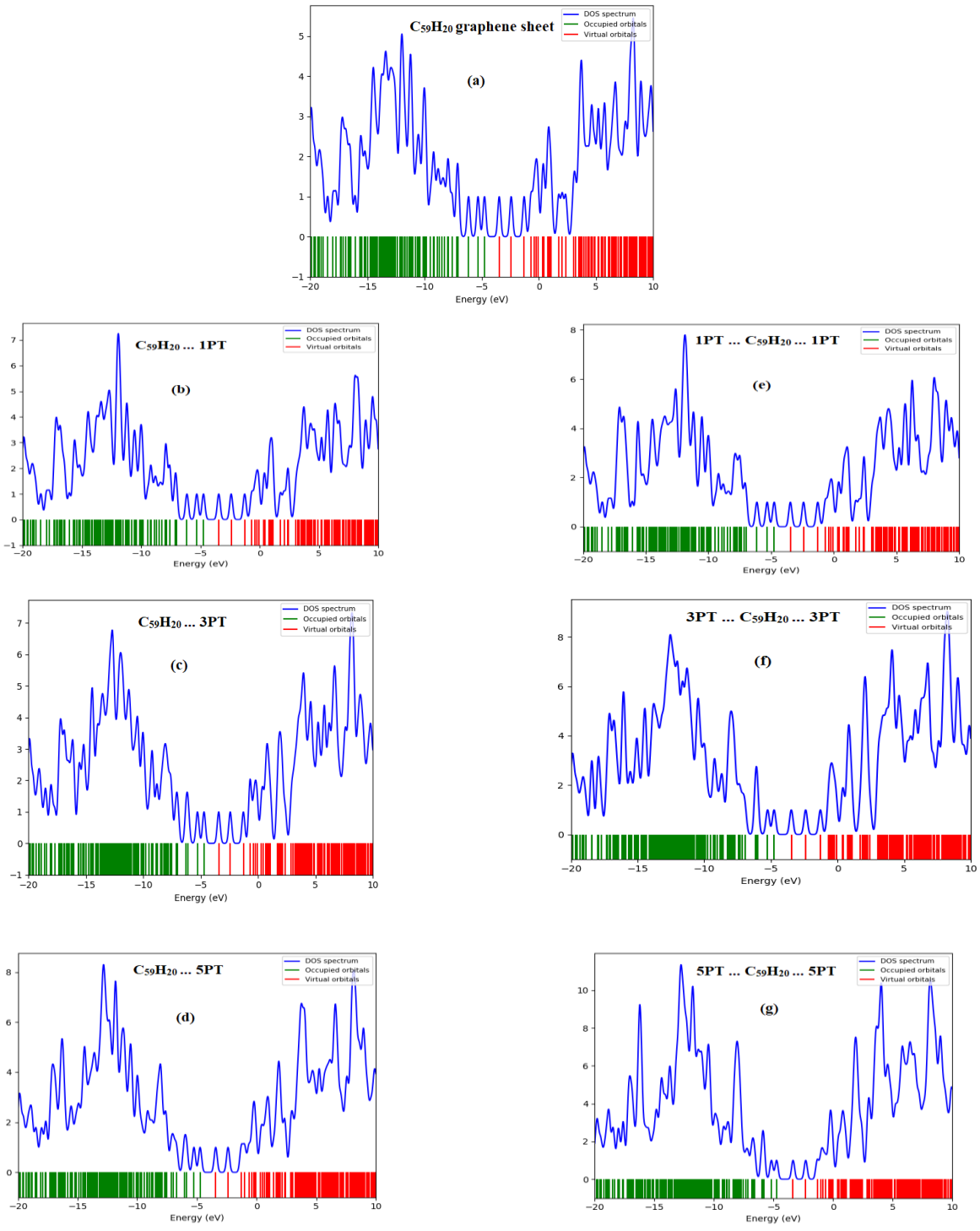

Figure S26: DOS spectra of (a) $C_{59}H_{20}$ (b) $C_{59}H_{20}$ ... 1PT, (c) $C_{59}H_{20}$ ... 3PT, (d) $C_{59}H_{20}$... 5PT, (e) 1PT… $C_{59}H_{20}$ ... 1PT, (f) 3PT… $C_{59}H_{20}$... 3PT, (g) 5PT… $C_{59}H_{20}$... 5PT composites

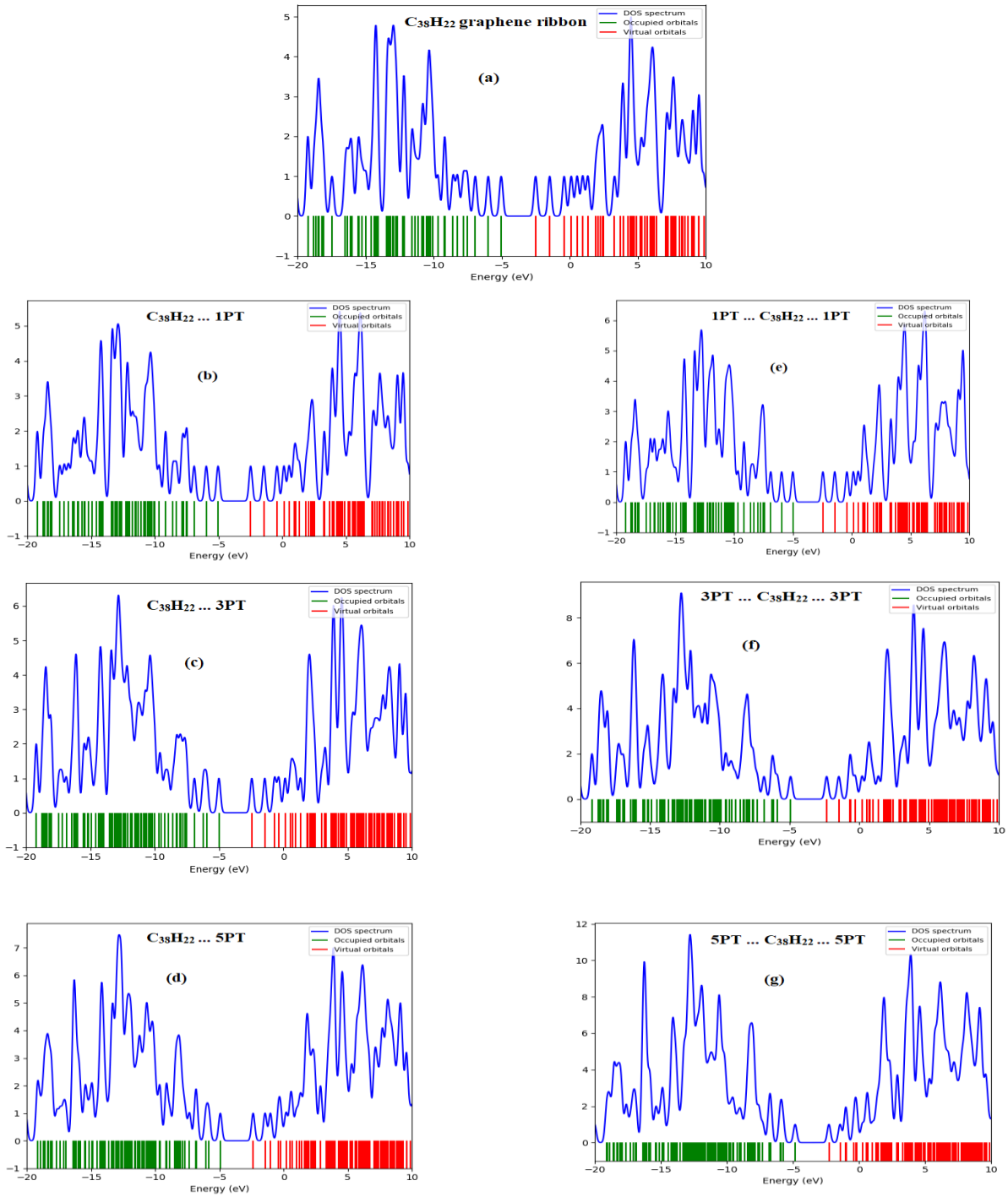

Figure S27: DOS spectra of (a) $C_{38}H_{22}$ (b) $C_{38}H_{22}$ ... 1PT, (c) $C_{38}H_{22}$ ... 3PT, (d) $C_{38}H_{22}$... 5PT, (e) 1PT… $C_{38}H_{22}$ ... 1PT, (f) 3PT… $C_{38}H_{22}$ ... 3PT, (g) 5PT… $C_{38}H_{22}$ ... 5PT composites

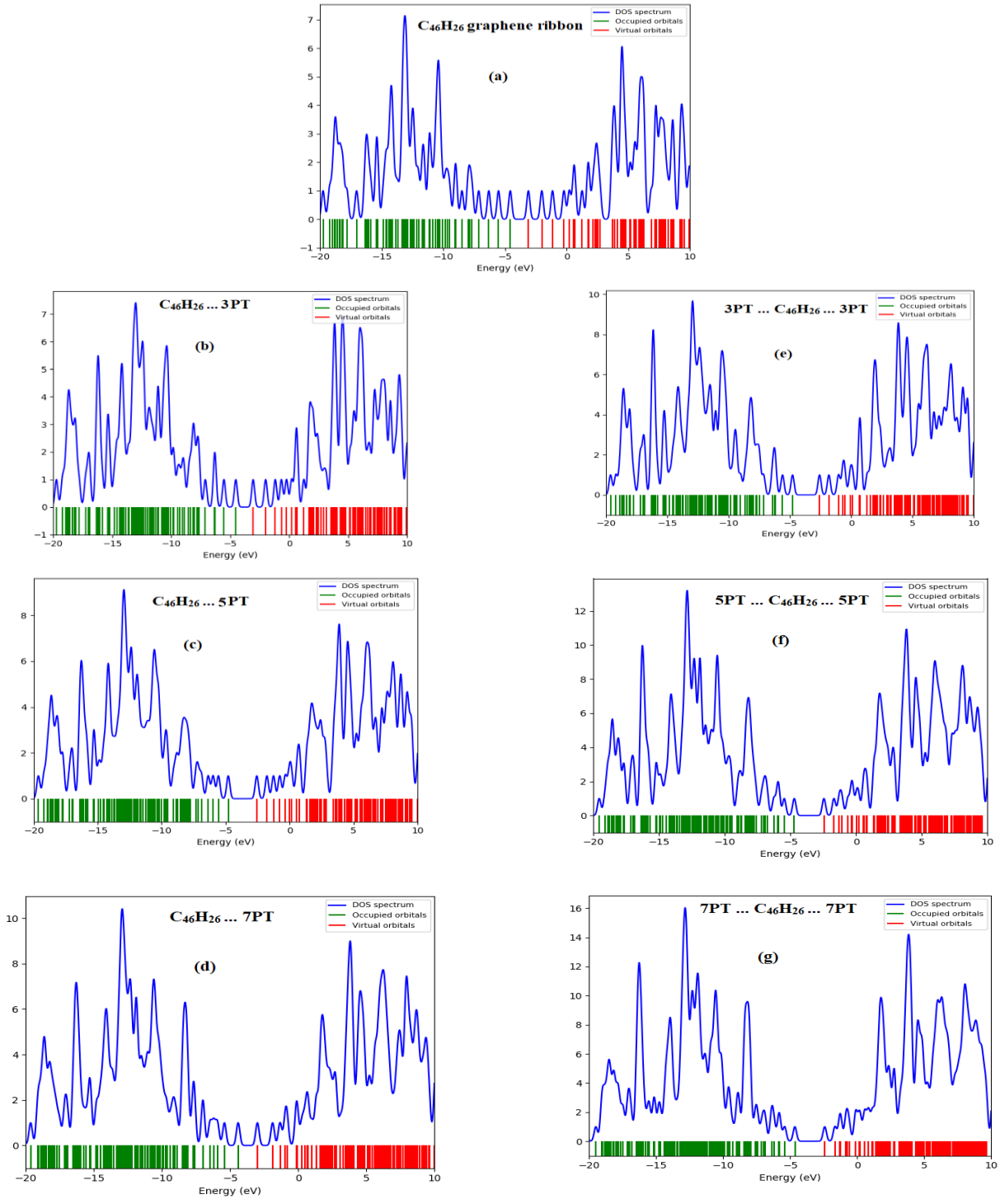

Figure S28: DOS spectra of (a) $C_{46}H_{26}$ (b) $C_{46}H_{26}$ ... 3PT, (c) $C_{46}H_{26}$ ... 5PT, (d) $C_{46}H_{26}$... 7PT, (e) 3PT… $C_{46}H_{26}$ ... 3PT, (f) 5PT… $C_{46}H_{26}$... 5PT, (g) 7PT… $C_{46}H_{26}$ ... 7PT composites

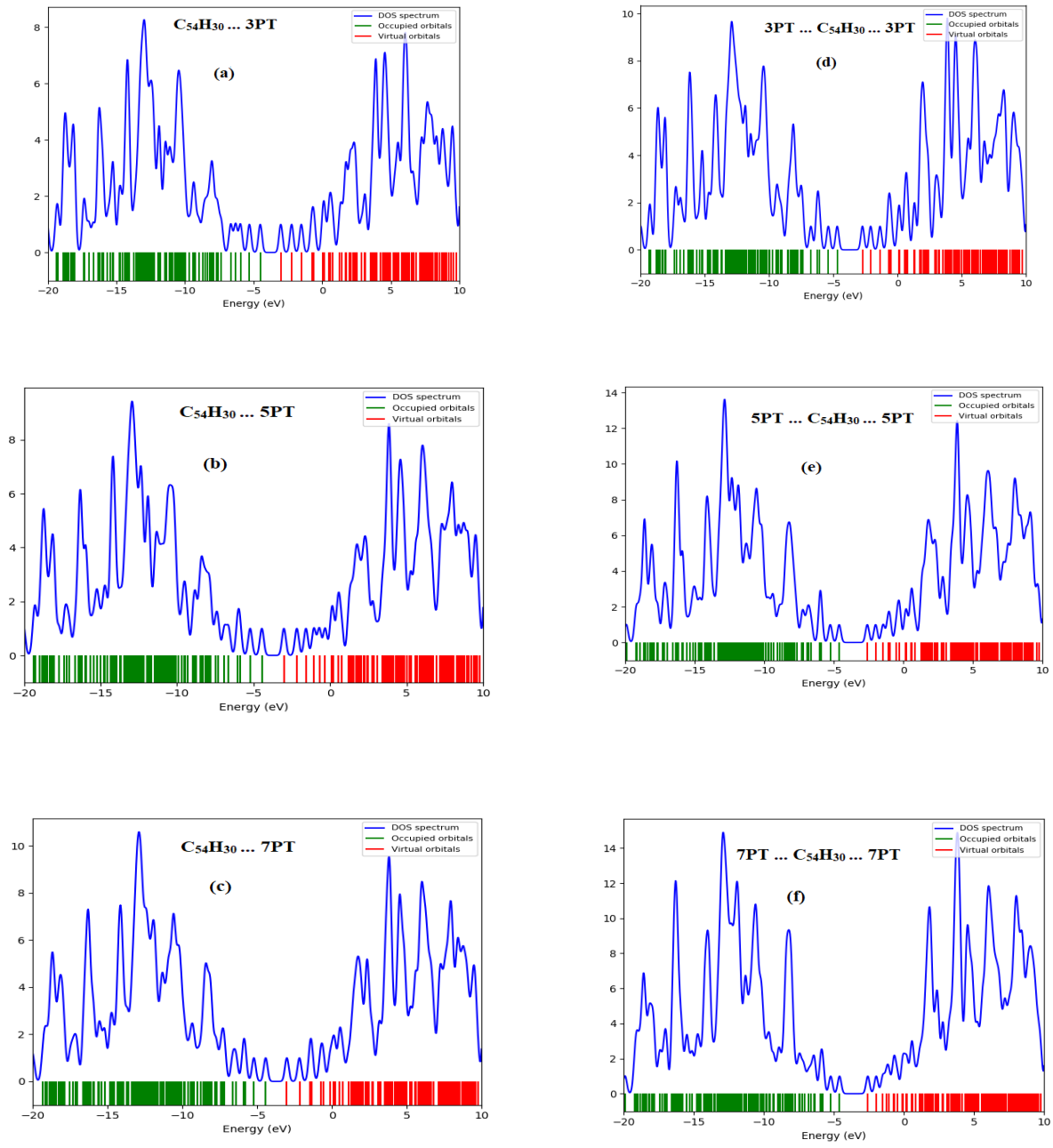

Figure S29: DOS spectra of (a) $C_{54}H_{30}$ ... 3PT, (b) $C_{54}H_{30}$ ... 5PT, (c) $C_{54}H_{30}$... 7PT, (d) 3PT… $C_{54}H_{30}$ ... 3PT, (e) 5PT… $C_{54}H_{30}$... 5PT, (f) 7PT… $C_{54}H_{30}$ ... 7PT composite

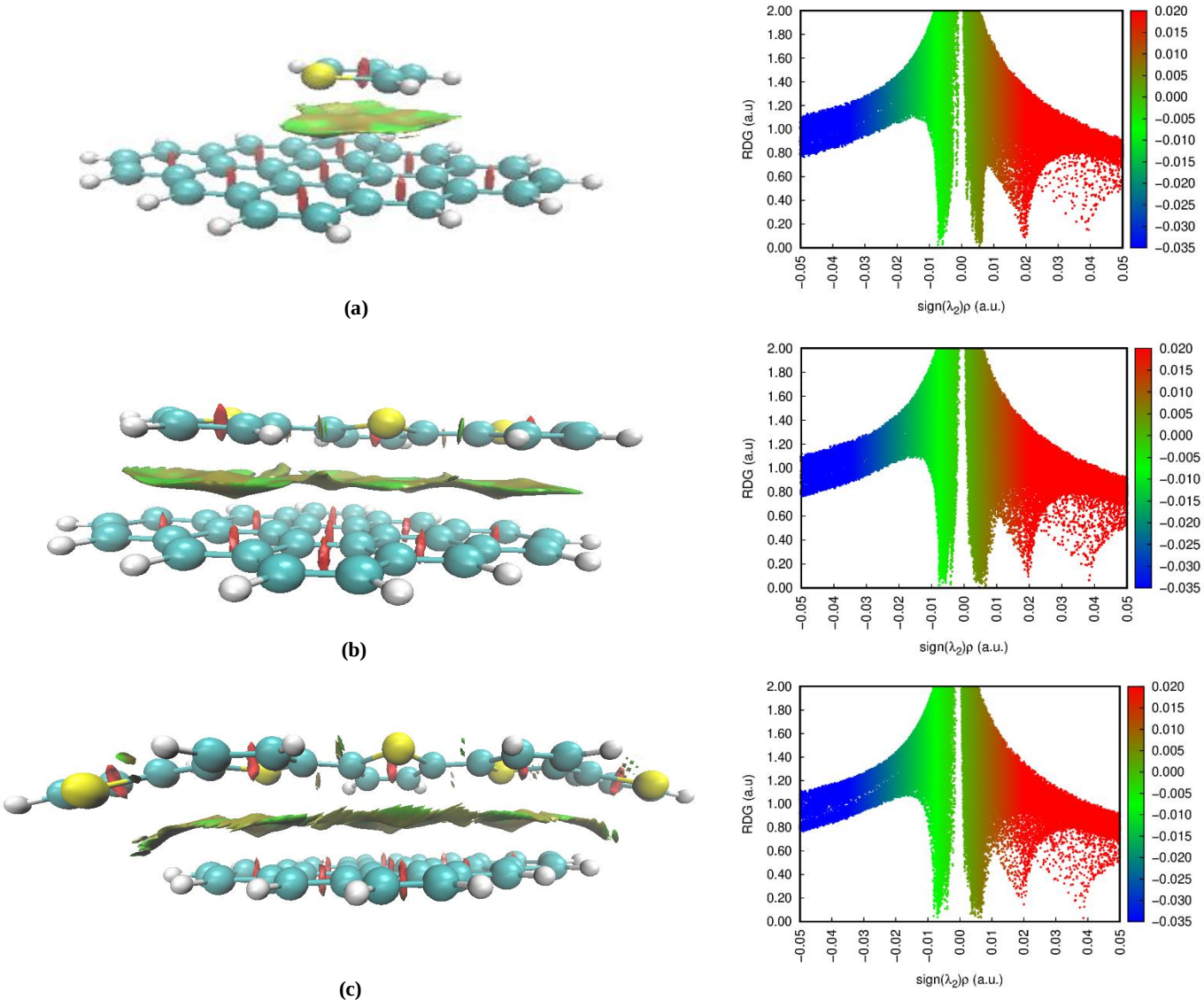

Figure S30: Color-mapped RDG isosurface graphs and scatter diagrams of (a) $C_{30}H_{14}$ ... 1PT, (b) $C_{30}H_{14}$ ... 3PT, (c) $C_{30}H_{14}$... 5PT composites

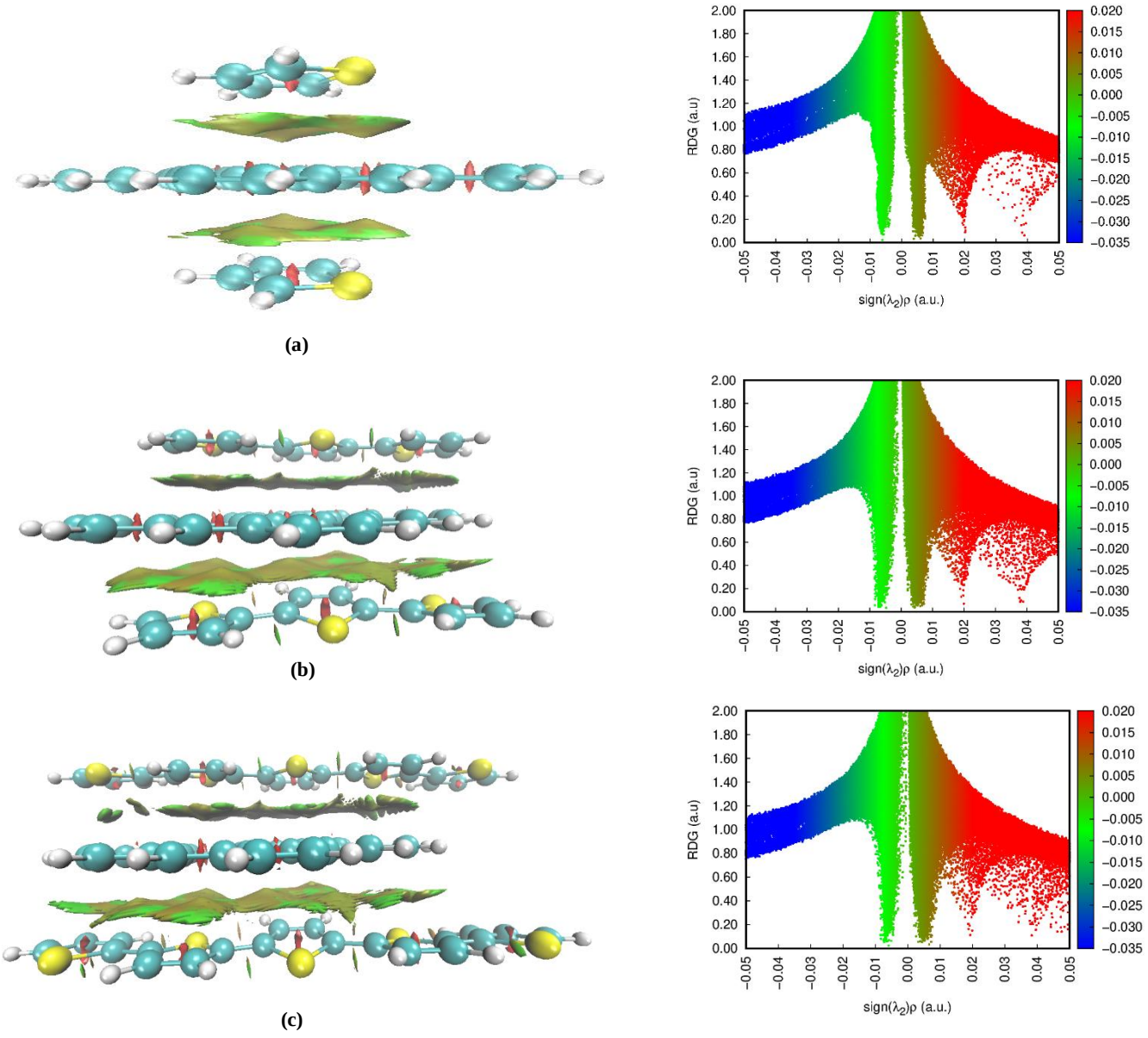

Figure S31: Color-mapped RDG isosurface graphs and scatter diagrams of (a) 1PT… $C_{30}H_{14}$ … 1PT, (b) 3PT… $C_{30}H_{14}$ … 3PT, (c) 5PT… $C_{30}H_{14}$ … 5PT composites

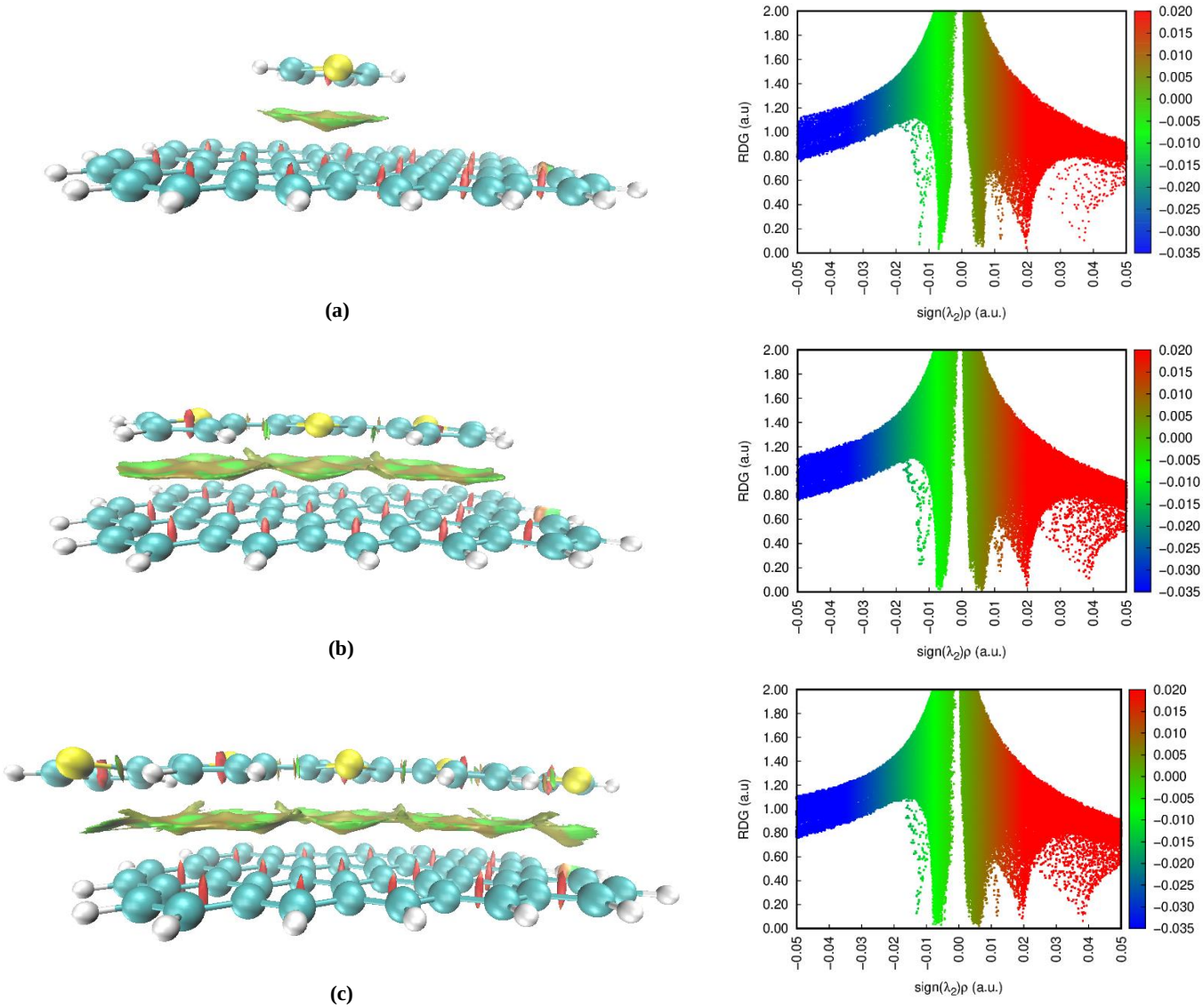

Figure S32: Color-mapped RDG isosurface graphs and scatter diagrams of (a) $C_{46}H_{18}$ ... 1PT, (b) $C_{46}H_{18}$ ... 3PT, (c) $C_{46}H_{18}$... 5PT composites

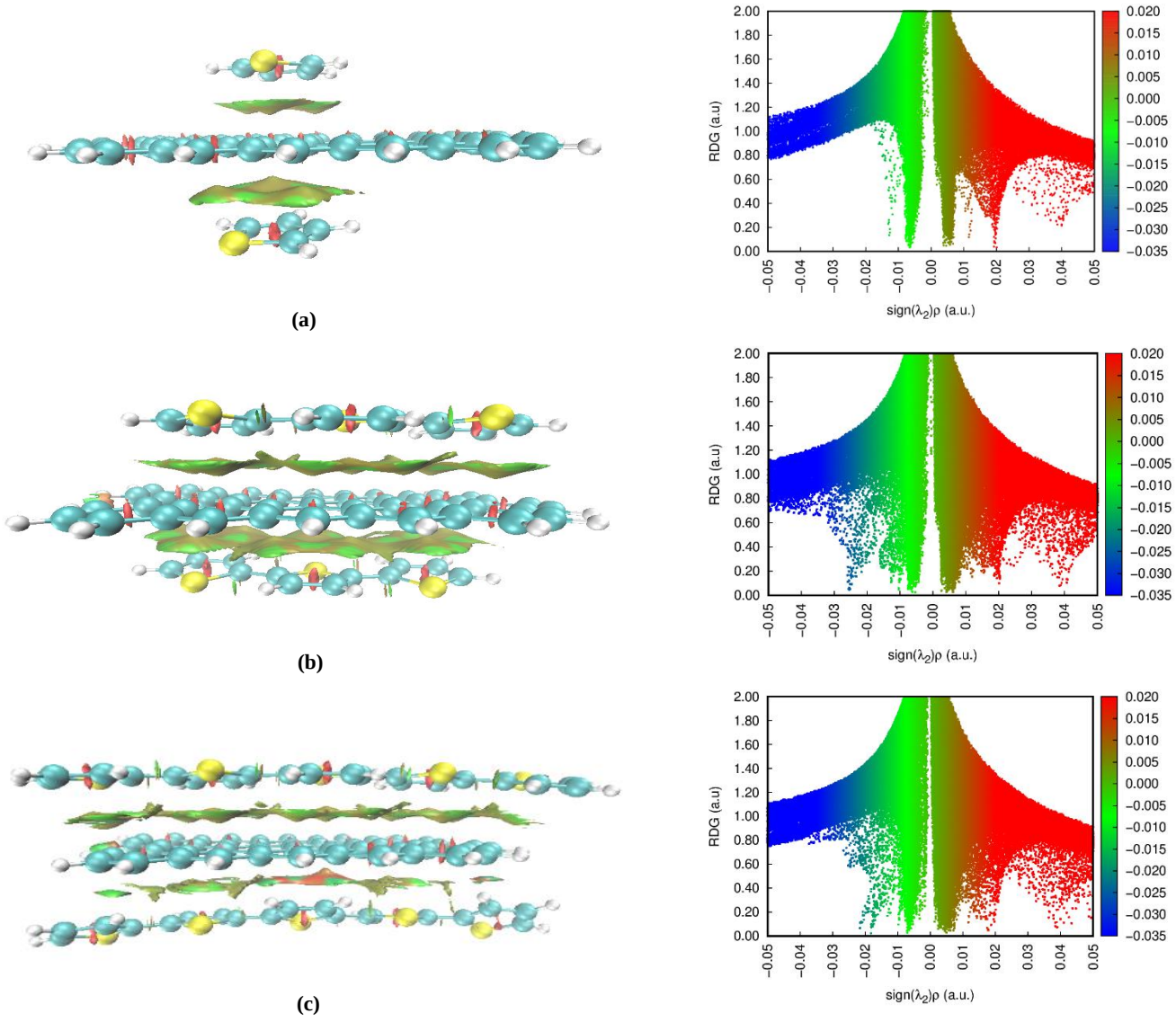

Figure S33: Color-mapped RDG isosurface graphs and scatter diagrams of (a) 1PT… $C_{46}H_{18}$ … 1PT, (b) 3PT… $C_{46}H_{18}$… 3PT, (c) 5PT… $C_{46}H_{18}$ … 5PT composites

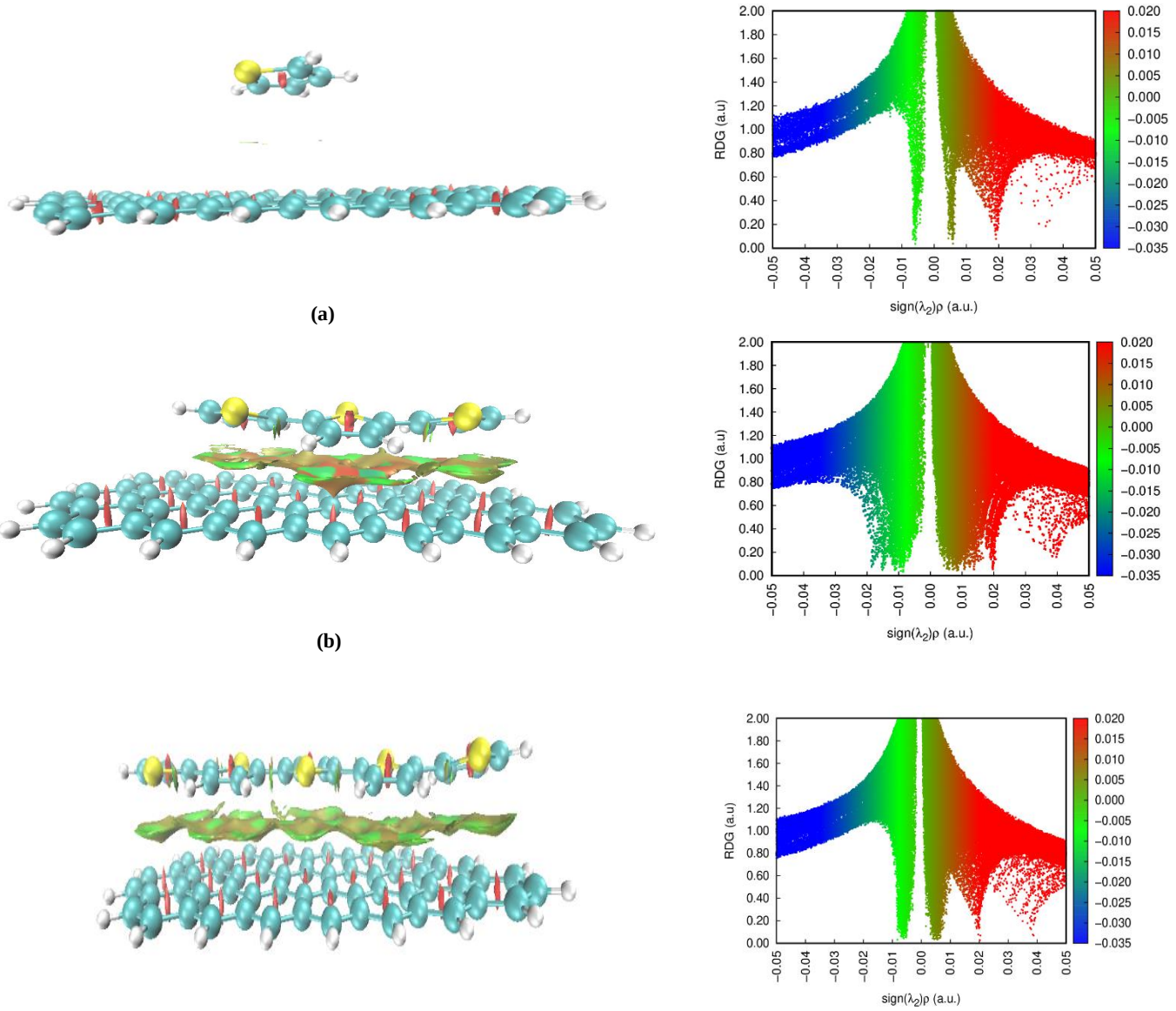

Figure S34: Color-mapped RDG isosurface graphs and scatter diagrams of (a) $C_{59}H_{20}$… 1PT, (b) 3PT… $C_{59}H_{20}$ and (c) 3PT… $C_{59}H_{20}$ composites

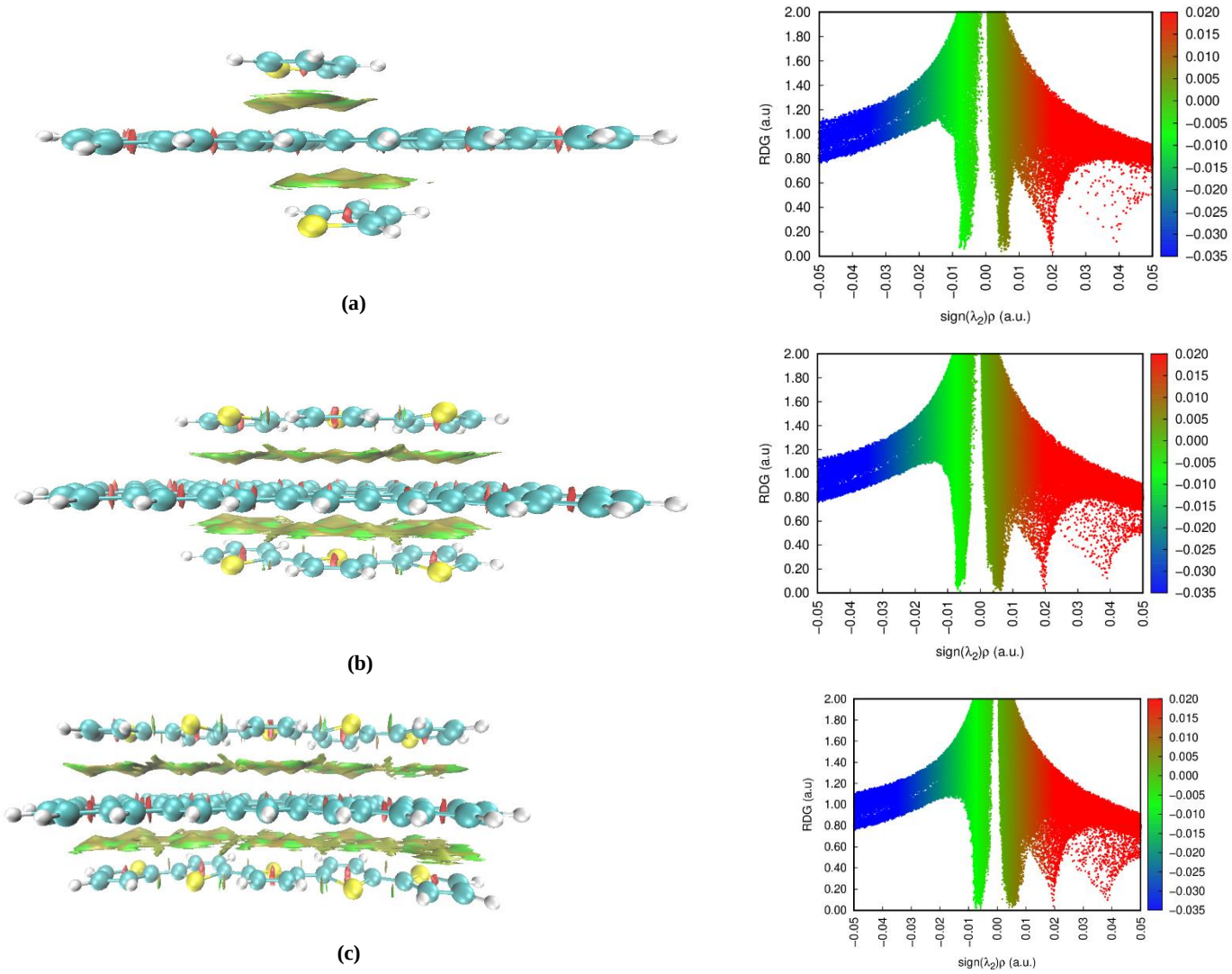

Figure S35: Color-mapped RDG isosurface graphs and scatter diagrams of (a) 1PT…$C_{59}H_{20}$… 1PT and (b) 3PT… $C_{59}H_{20}$... 3PT and (c) 5PT…$C_{59}H_{20}$… 5PT composites

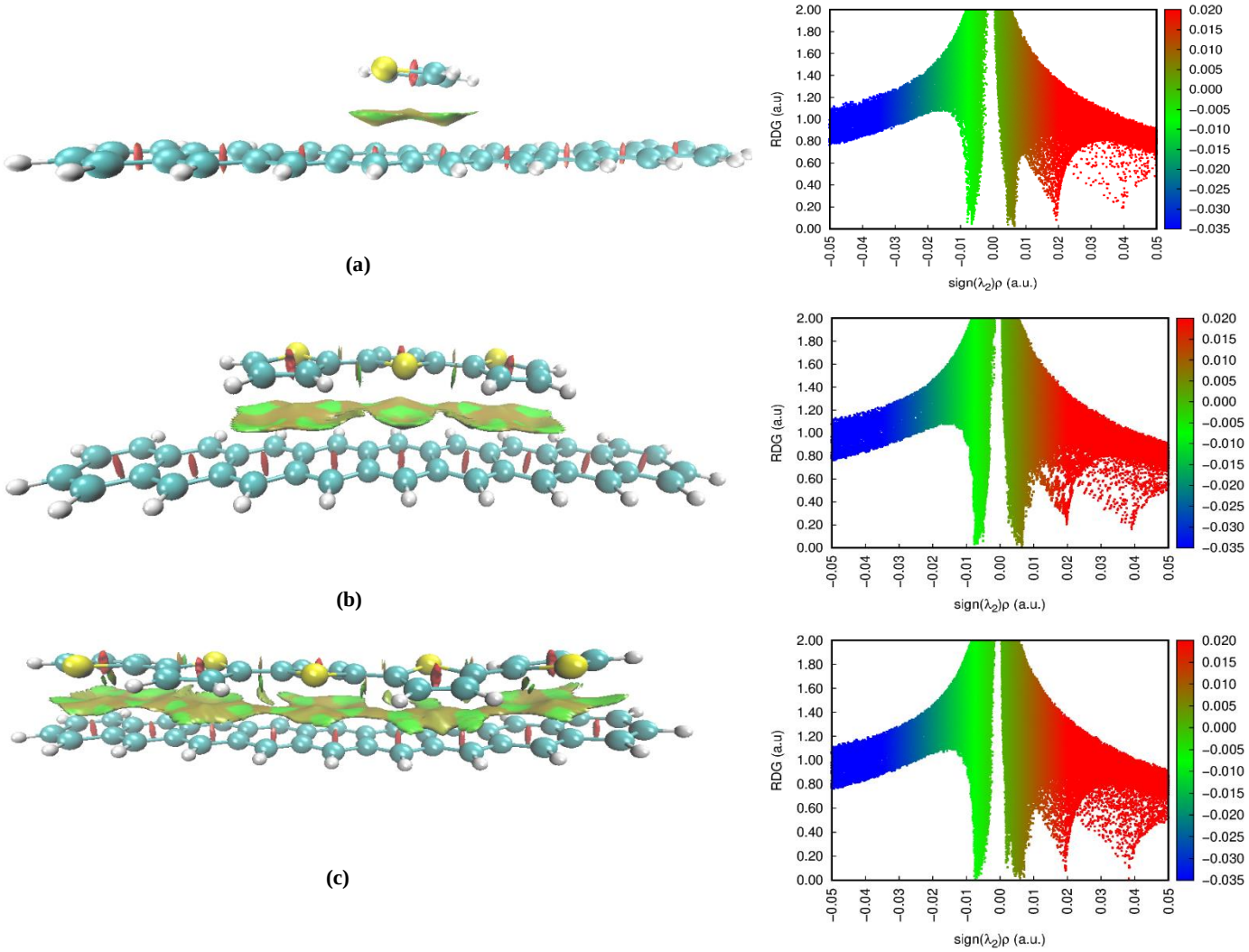

Figure S36: Color-mapped RDG isosurface graphs and scatter diagrams of (a) $C_{38}H_{22}$ ... 1PT, (b) $C_{38}H_{22}$... 3PT, (c) $C_{38}H_{22}$ ... 5PT composites

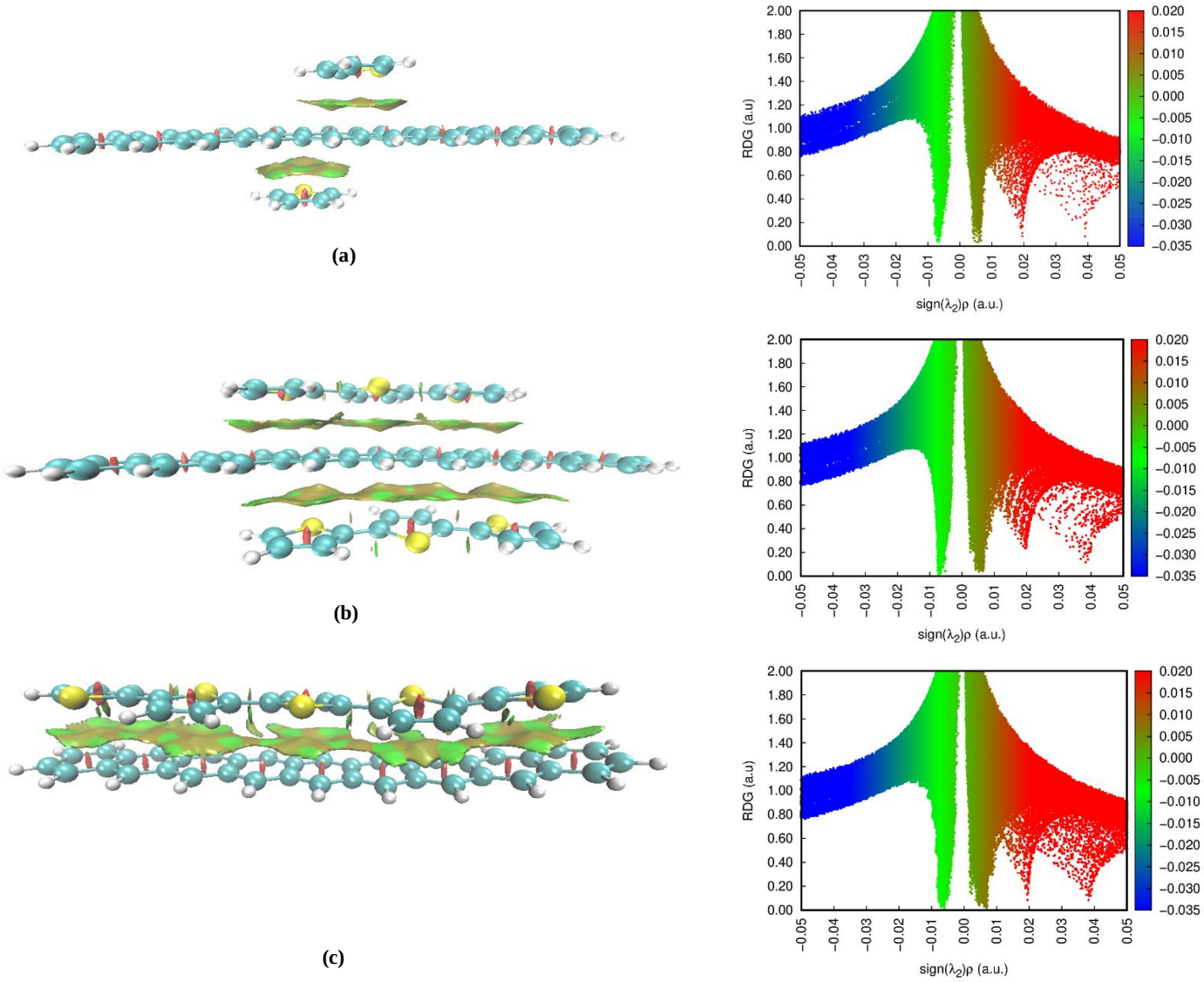

Figure S37: Color-mapped RDG isosurface graphs and scatter diagrams of (a) 1PT…$C_{38}H_{22}$ ... 1PT, (b) 3PT… $C_{38}H_{22}$... 3PT, (c) 5PT… $C_{38}H_{22}$ ... 5PT composites

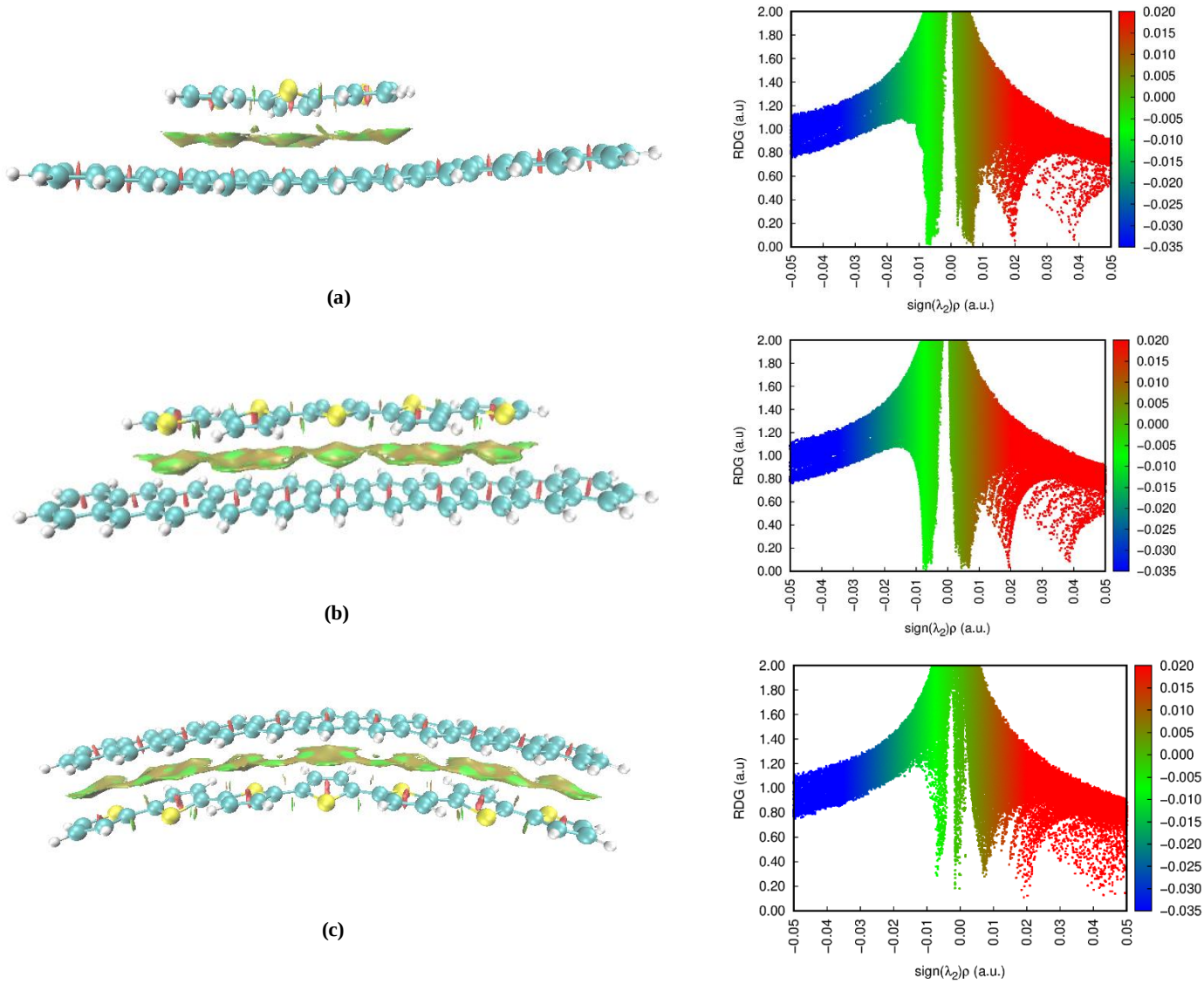

Figure S38: Color-mapped RDG isosurface graphs and scatter diagrams of (a) $C_{46}H_{26}$ ... 3PT, (b) $C_{46}H_{26}$... 5PT, (c) $C_{46}H_{26}$ ... 7PT composites

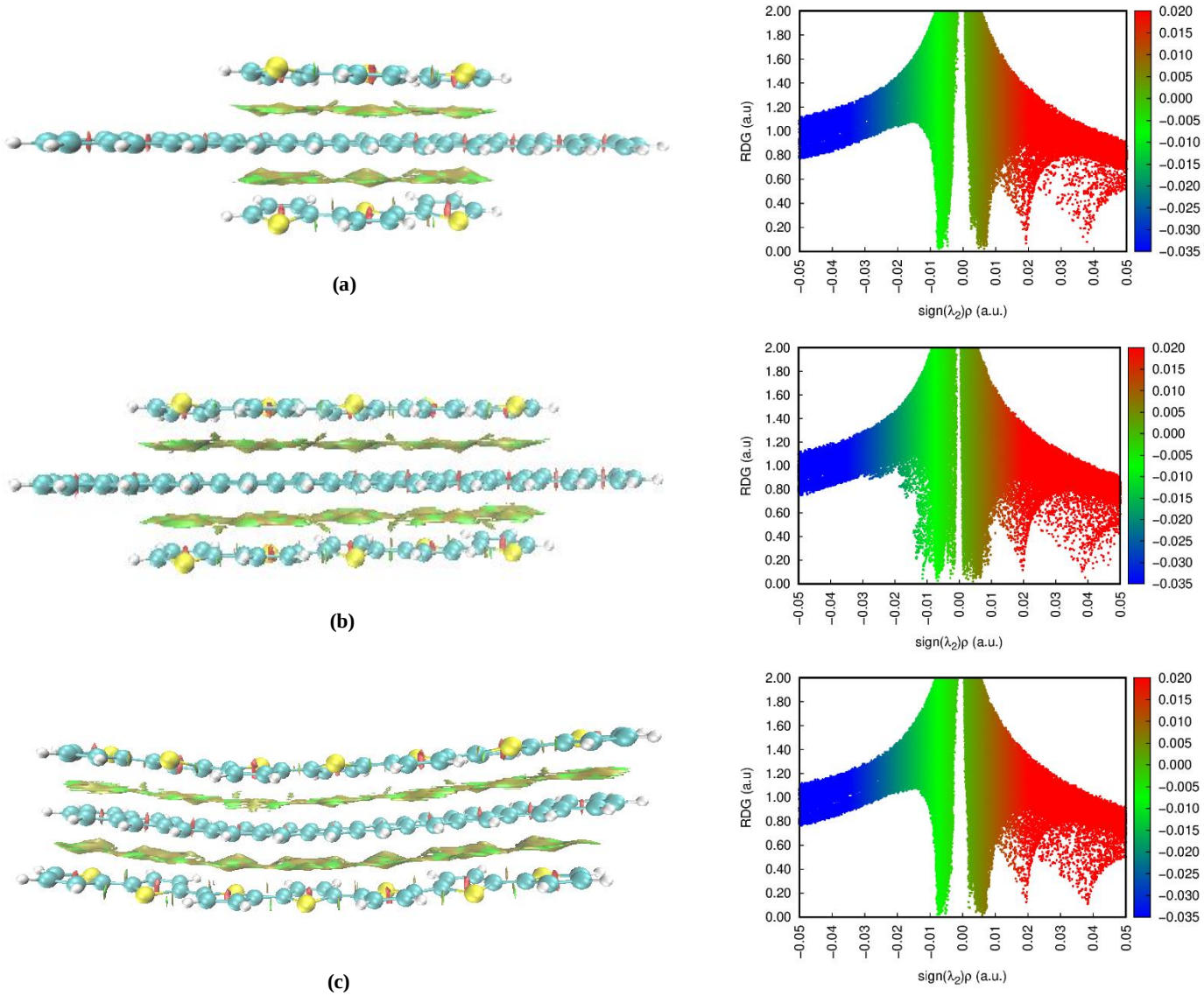

Figure S39: Color-mapped RDG isosurface graphs and scatter diagrams of (a) 3PT… $C_{46}H_{26}$ ... 3PT, (b) 5PT… $C_{46}H_{26}$... 5PT, (c) 7PT… $C_{46}H_{26}$ ... 7PT composites

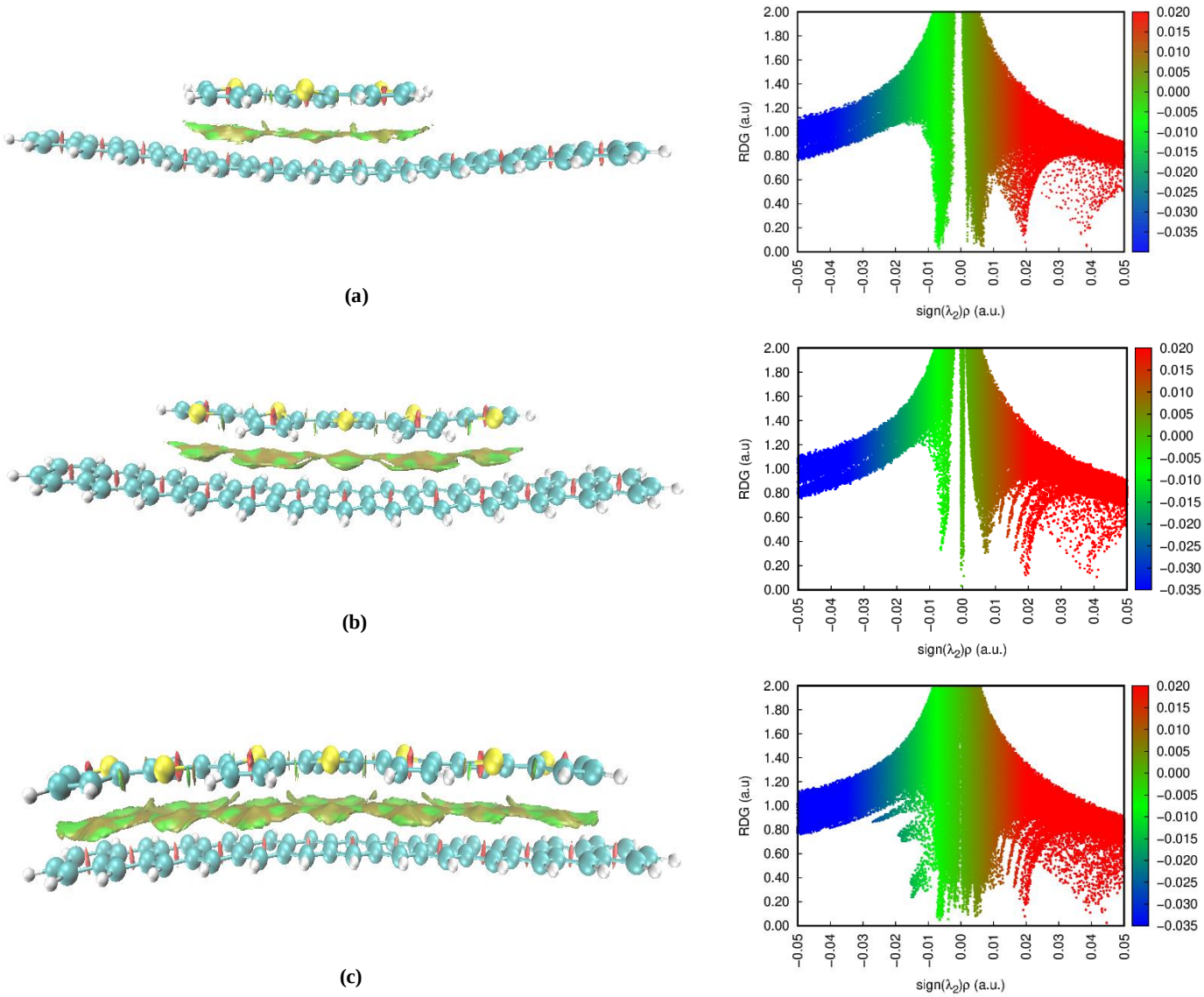

Figure S40: Color-mapped RDG isosurface graphs and scatter diagrams of (a) $C_{54}H_{30}$ ... 3PT, (b) $C_{54}H_{30}$... 5PT, (c) $C_{54}H_{30}$ ... 7PT composites

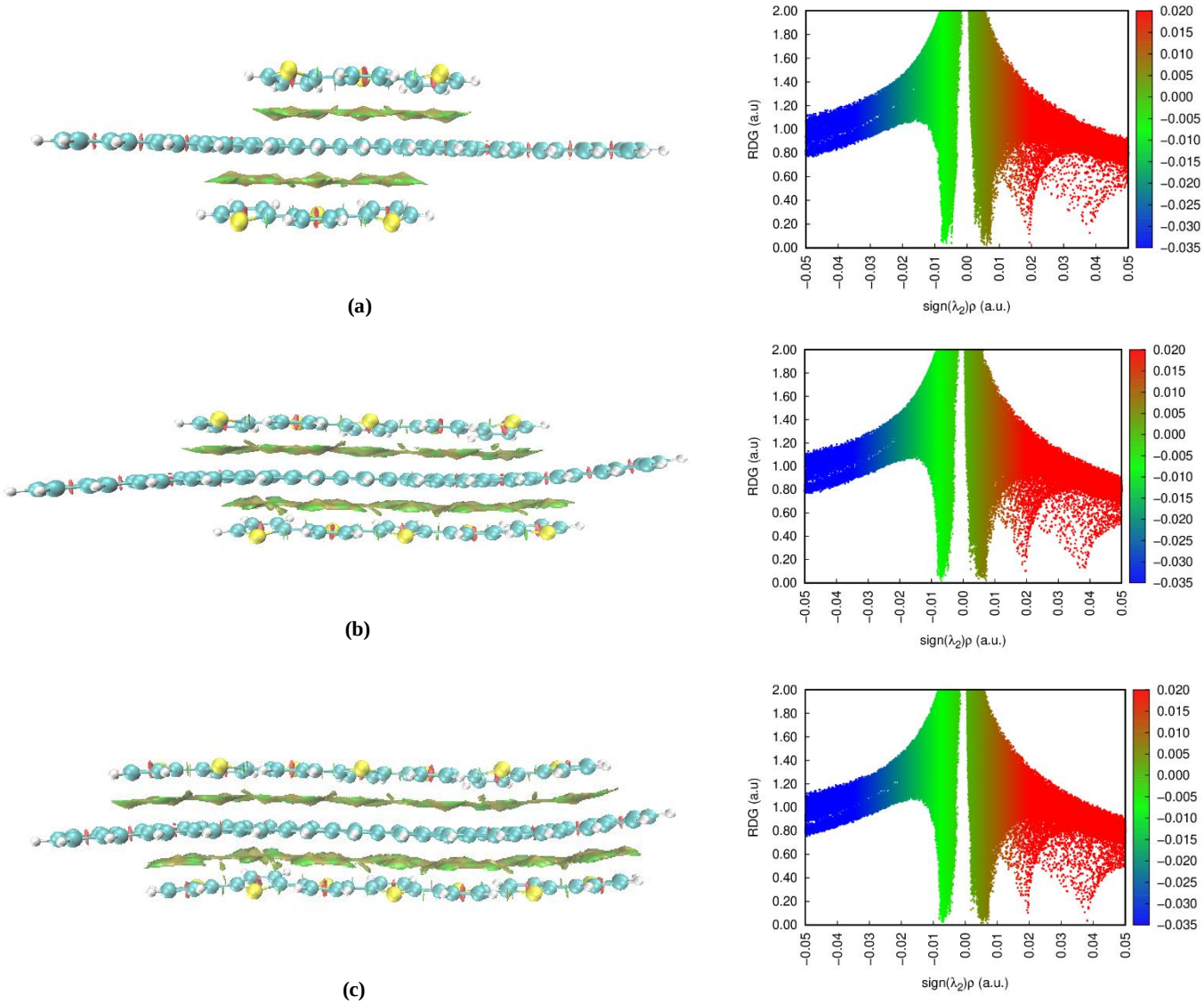

Figure S41: Color-mapped RDG isosurface graphs and scatter diagrams of (a) 3PT… $C_{54}H_{30}$ … 3PT, (b) 5PT… $C_{54}H_{30}$… 5PT, (c) 7PT… $C_{54}H_{30}$ … 7PT composites