Supporting Information

Electronic structure of polypyrrole composited with low percent of graphene nanofiller

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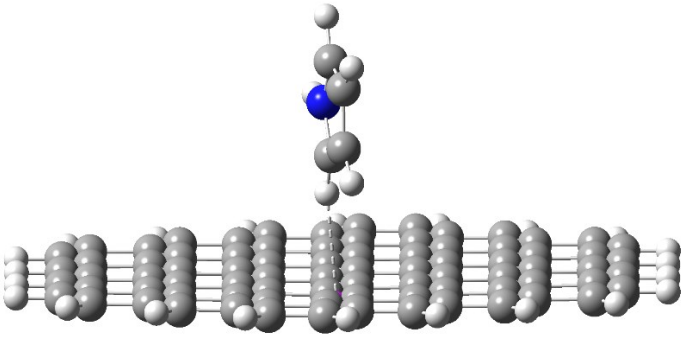
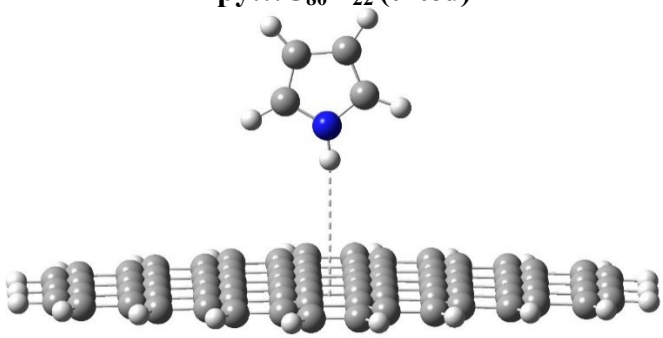
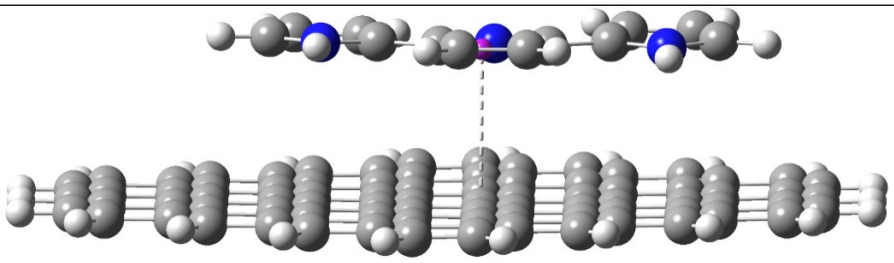


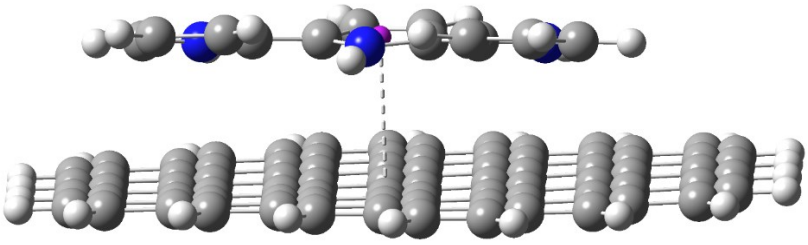
1py…$C_{80}H_{22}$ (tilted)



1Py…$C_{80}H_{22}$ (vertical)

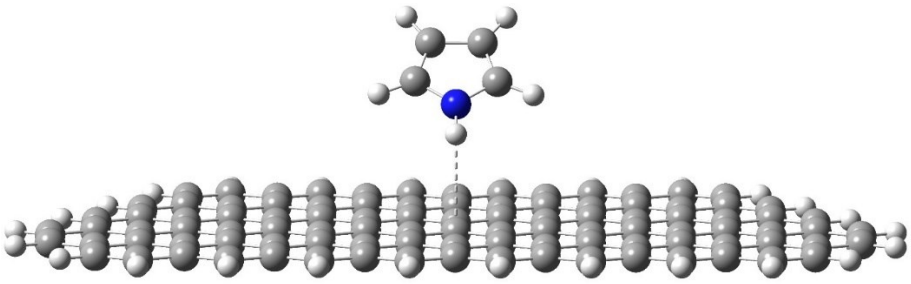


3Py…$C_{80}H_{22}$ (titled)

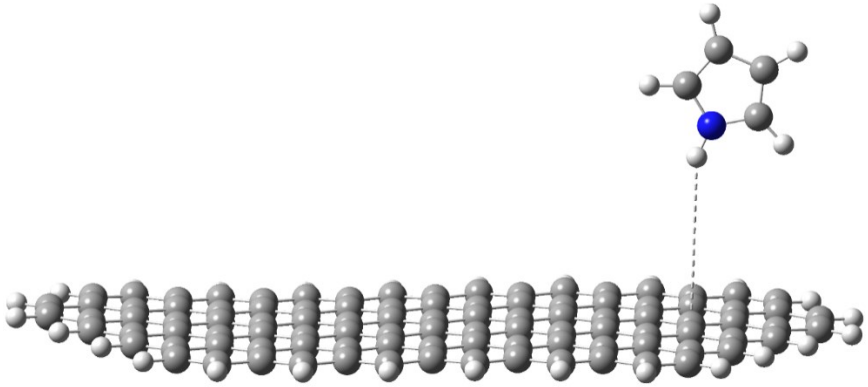


3Py…$C_{80}H_{22}$ (vertical)

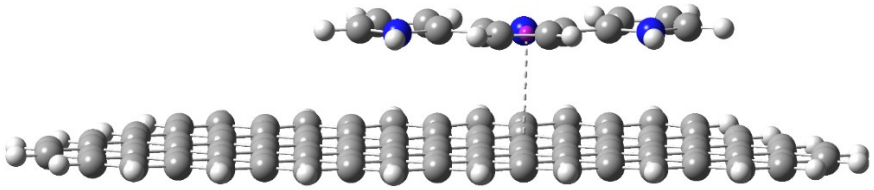
Figure S1. Optimized configuration of titled and vertical $C_{80}H_{22}$…nPy composite.



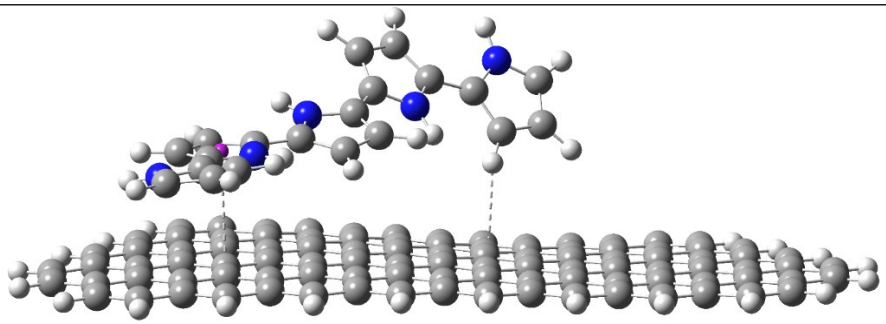
1Py…$C_{100}H_{26}$ (titled)



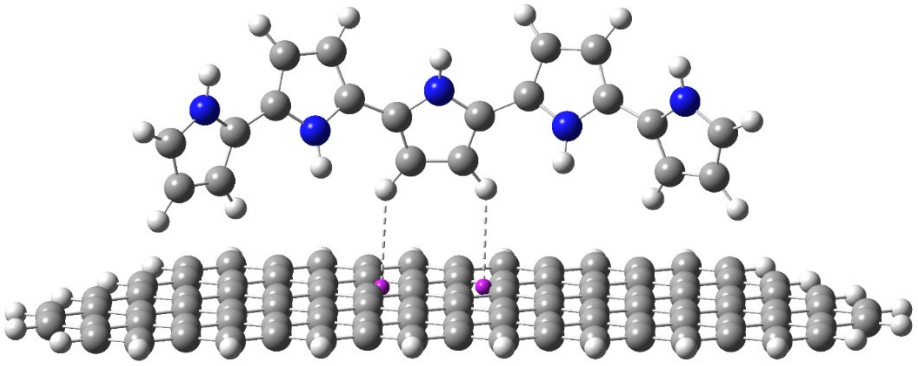
1Py…$C_{100}H_{26}$ (vertical)



3Py…$C_{100}H_{26}$ (titled)

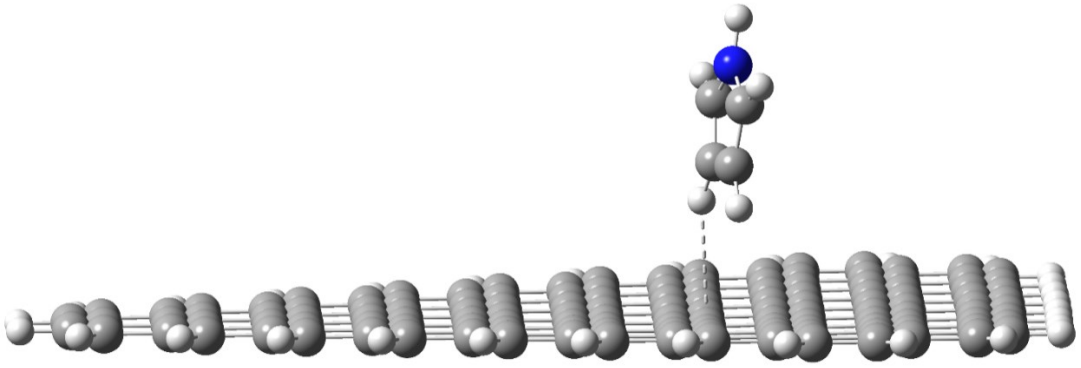


5Py…$C_{100}H_{26}$ (titled)

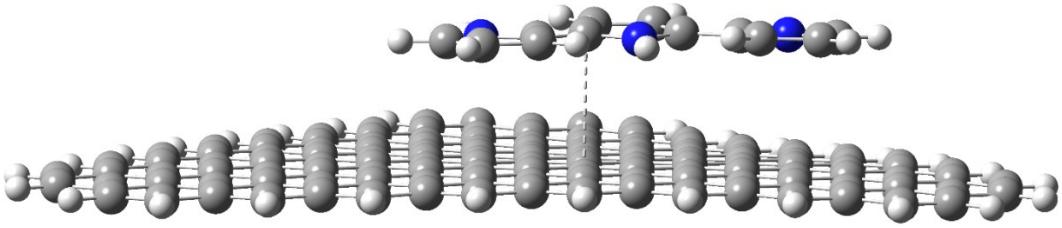


5Py@$C_{100}H_{26}$ (vertical)

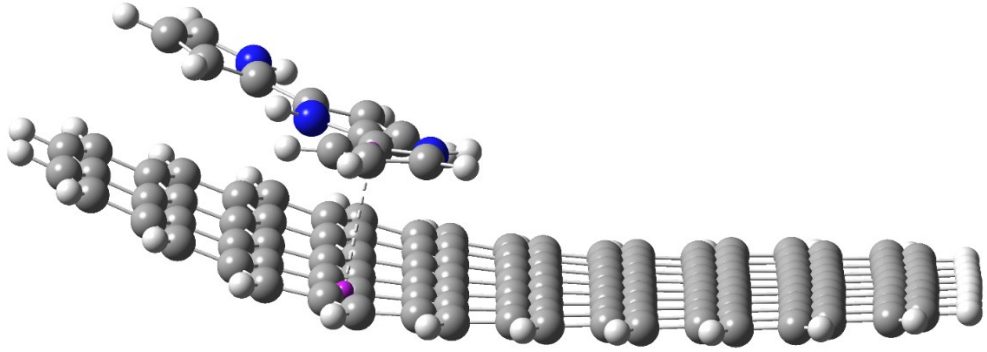
Figure S2. Optimized configuration of vertical $C_{100}H_{26}$…nPy composite



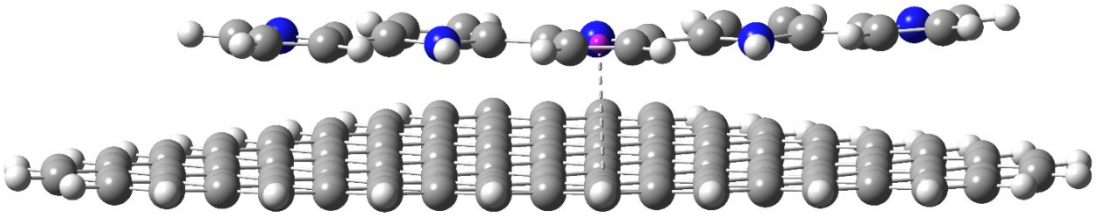
1Py@$C_{132}H_{30}$ (vertical)



3Py@$C_{132}H_{30}$ (titled)

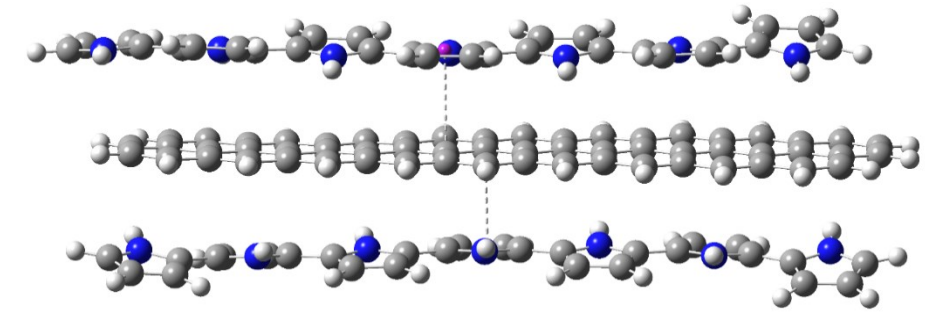


3Py@$C_{132}H_{30}$ (vertical)

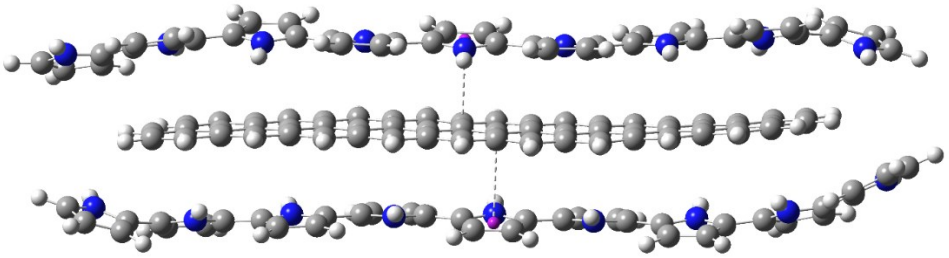


5Py@$C_{132}H_{30}$ (tilted)

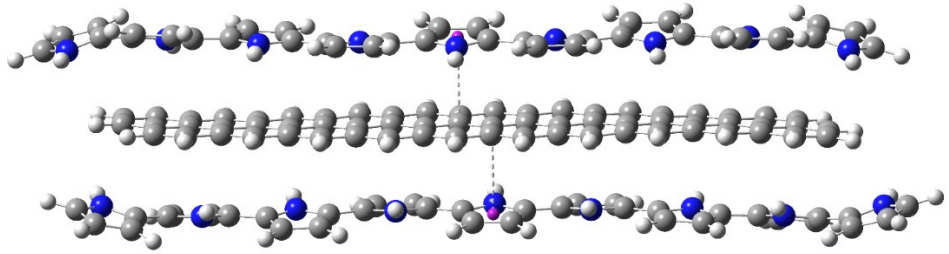
Figure S3. Optimized configuration of tilted and vertical $C_{132}H_{30}$…nPy composites



7Py…$C_{58}H_{24}$…7Py



9Py…$C_{58}H_{24}$…9Py



9Py…$C_{64}H_{26}$…9Py

Figure S3. Optimized configuration of nPy…$C_{58}H_{24}$…nPy and nPy…$C_{64}H_{26}$…nPy composites

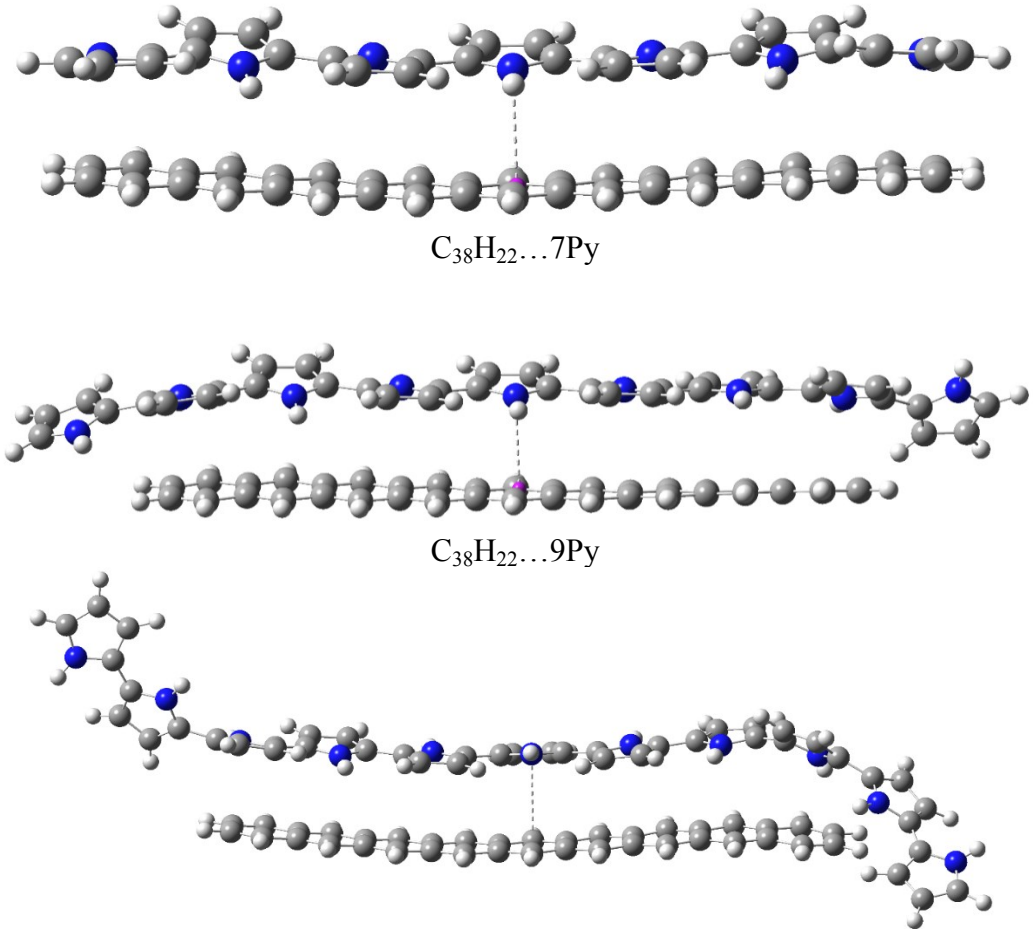
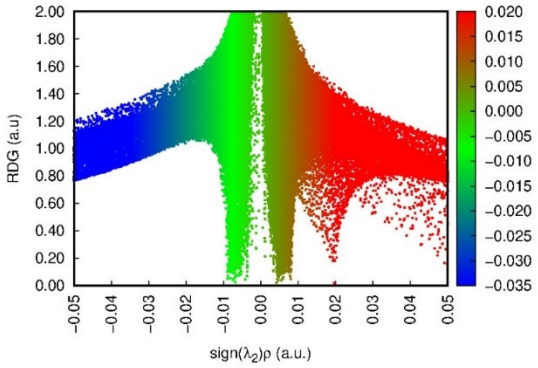
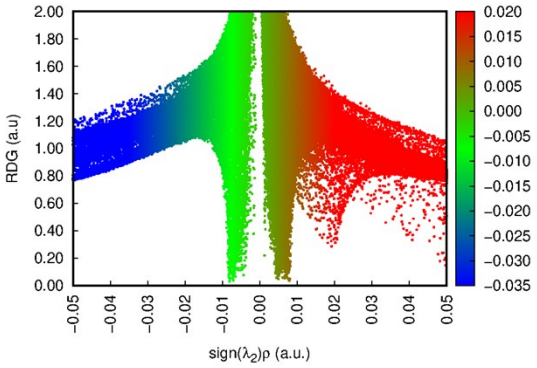


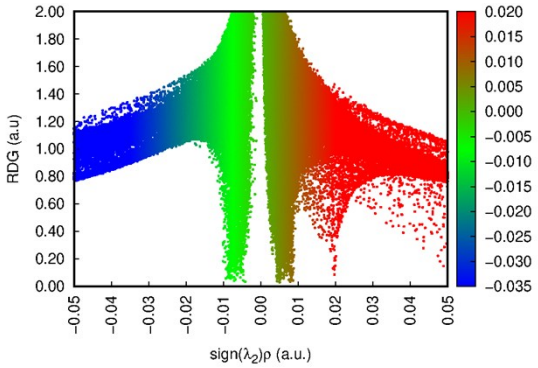
Figure S4. Optimized configuration of $C_{38}H_{22}$…nPy composites



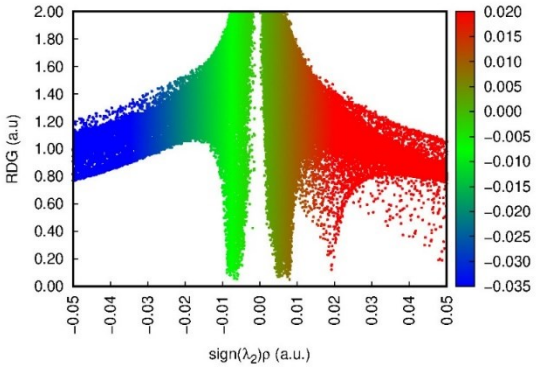
$C_{58}H_{24}$…11Py



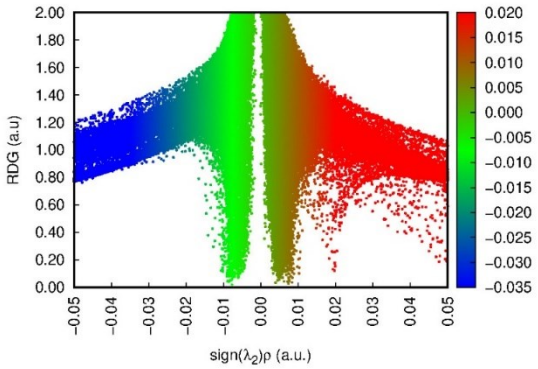
$C_{58}H_{24}$…13Py



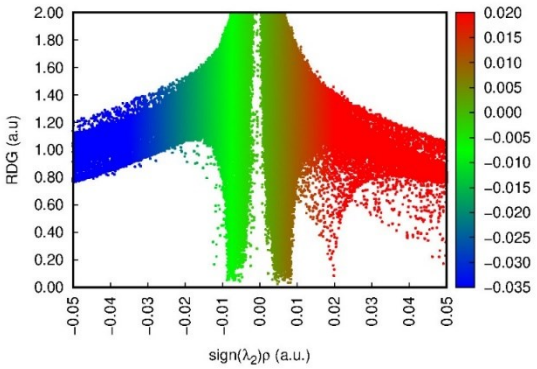
$C_{64}H_{26}$…11Py



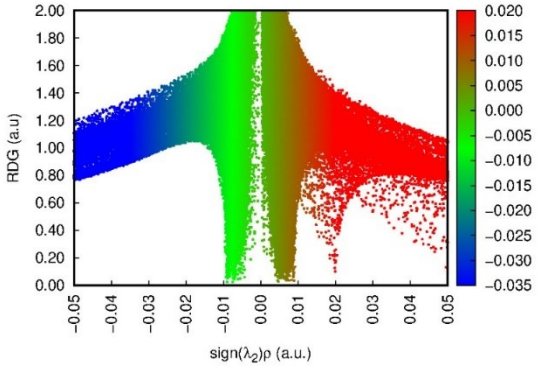
$C_{64}H_{26}$…13Py



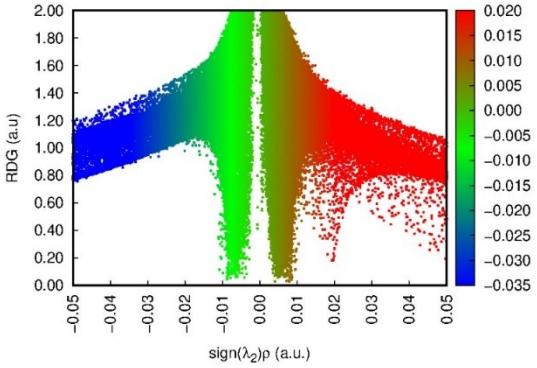
11Py…$C_{58}H_{24}$…11Py



13Py…$C_{58}H_{24}$…13Py



11Py…$C_{64}H_{26}$…11Py



13Py…$C_{64}H_{26}$…13Py

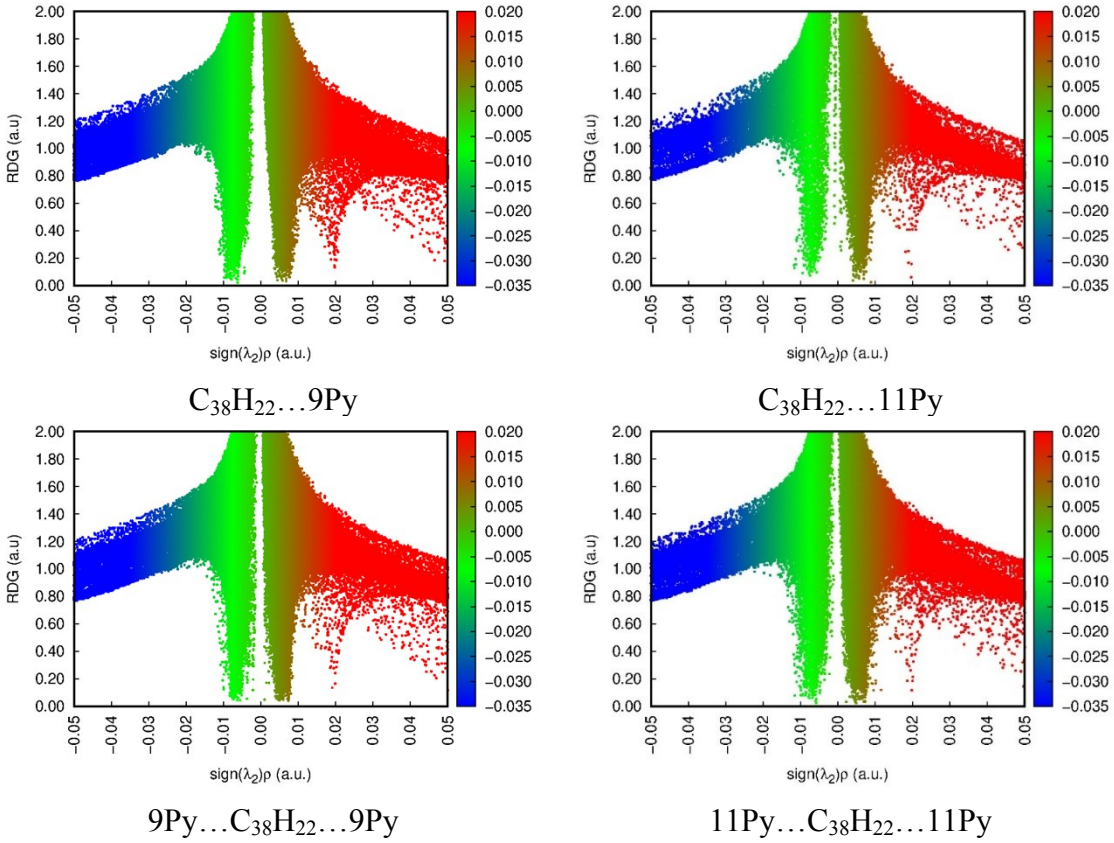
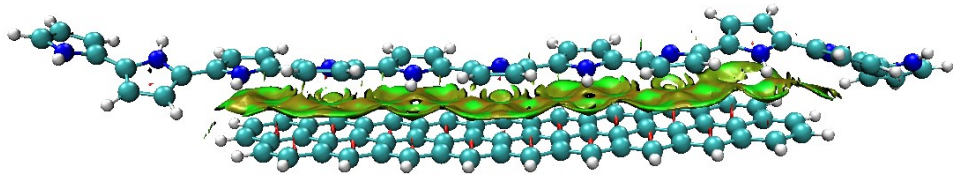
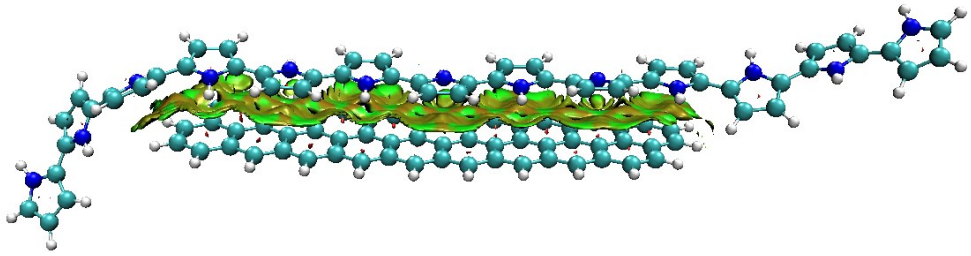


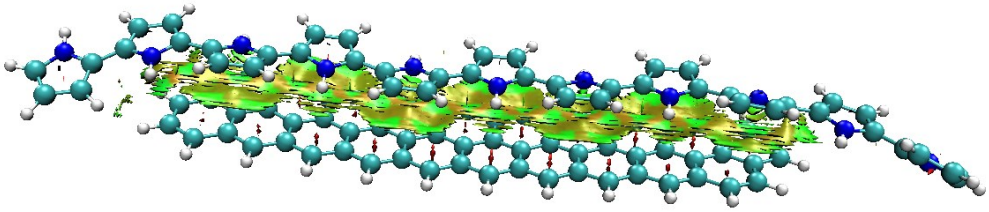
Figure S5. Isosurface 2D RDG scatter graph at isovalue of o.5 a.u. of polypyrrole/graphene composite.



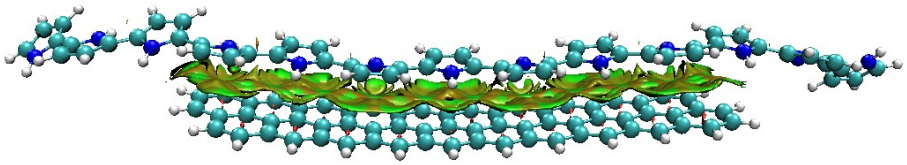
$C_{58}H_{24}$...11Py



$C_{58}H_{24}$...13Py

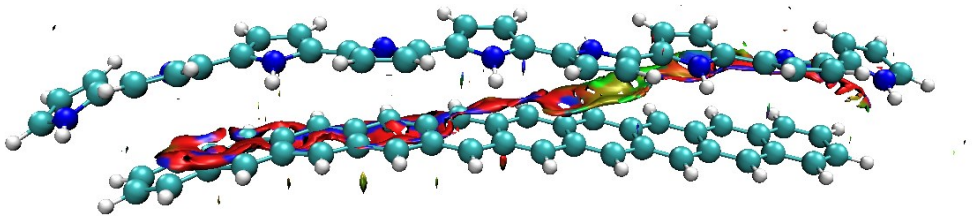


$C_{64}H_{26}$...11Py

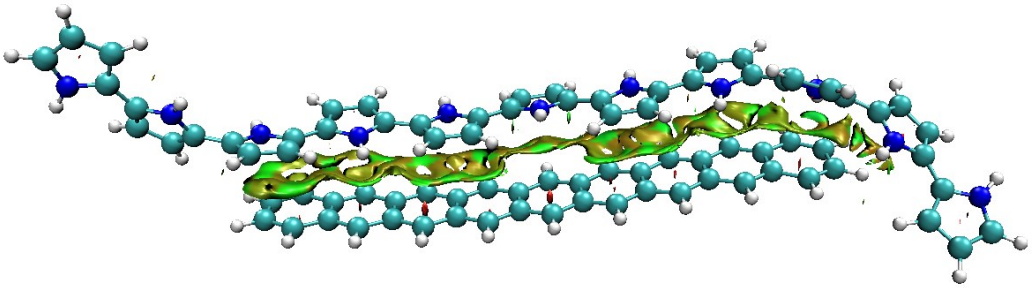


$C_{64}H_{26}$...13Py

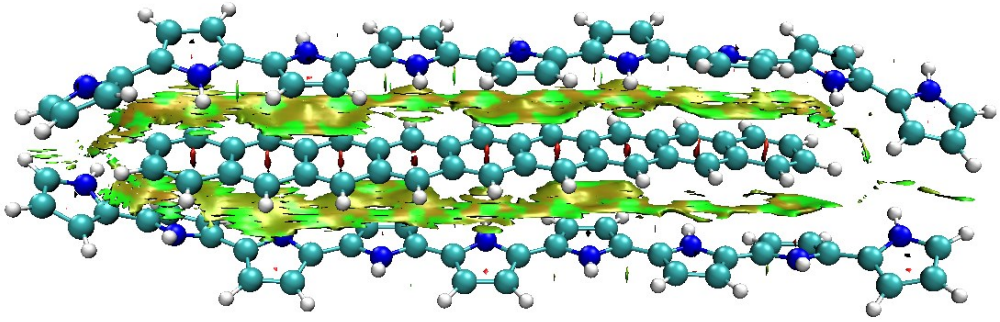
Figure S6. NCI analysis of optimized geometries of $C_{58}H_{24}$ and $C_{64}H_{26}$…nPy composite with isosruface value of 0.5 a.u.



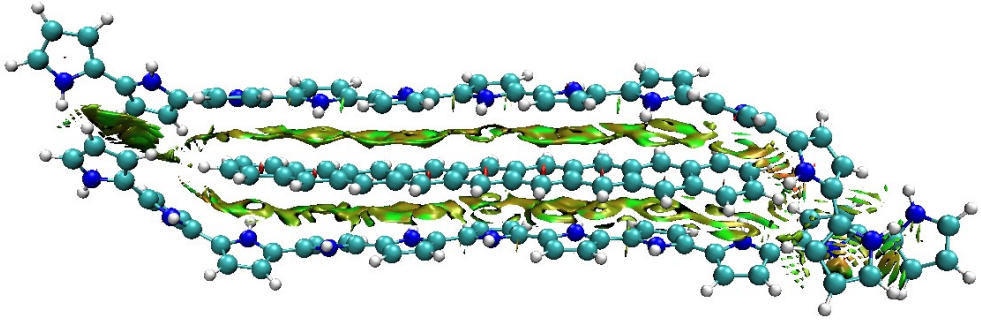
$C_{38}H_{22}$…9Py



$C_{38}H_{22}$…11Py



9Py… $C_{38}H_{22}$…9Py



11Py…$C_{38}H_{22}$…11Py

Figure 7. NCI analysis of optimized geometries of nPy…$C_{38}H_{22}$ and nPy…$C_{38}H_{22}$…nPy composite with isosruface value of 0.5 a.u.

Table S1: Values of BCPs parameters of $C_{80}H_{22}$ ...1Py and $C_{80}H_{22}$ ...3Py composites resulted through QTAIM analysis.

Composite	CP #	ρ	∇2ρ	G (r)	V (r)	H (r)	Eint
$C_{80}H_{22}$---1Py	1	0.00620	0.01904	0.00393	-0.00311	0.00083	-0.98
	2	0.00659	0.01996	0.00436	-0.00373	0.00063	-1.17
	3	0.00583	0.01658	0.00345	-0.00276	0.00069	-0.86
	4	0.00493	0.01441	0.00296	-0.00231	0.00065	-0.72
$C_{80}H_{22}$---3Py	1	0.00528	0.01653	0.00355	-0.00298	0.00058	-0.93
	2	0.00699	0.02015	0.00420	-0.00337	0.00084	-1.06
	3	0.00649	0.02036	0.00416	-0.00322	0.00093	-1.01
	4	0.00620	0.01753	0.00367	-0.00296	0.00071	-0.93
	5	0.00623	0.01786	0.00371	-0.00295	0.00076	-0.93
	6	0.00648	0.02086	0.00430	-0.00339	0.00091	-1.06
	7	0.00647	0.02033	0.00439	-0.00370	0.00069	-1.16
	8	0.00668	0.01910	0.00395	-0.00312	0.00083	-0.98
	9	0.00678	0.01987	0.00409	-0.00321	0.00088	-1.01
	10	0.00665	0.02006	0.00441	-0.00381	0.00060	-1.20
	11	0.00686	0.01978	0.00411	-0.00327	0.00084	-1.03

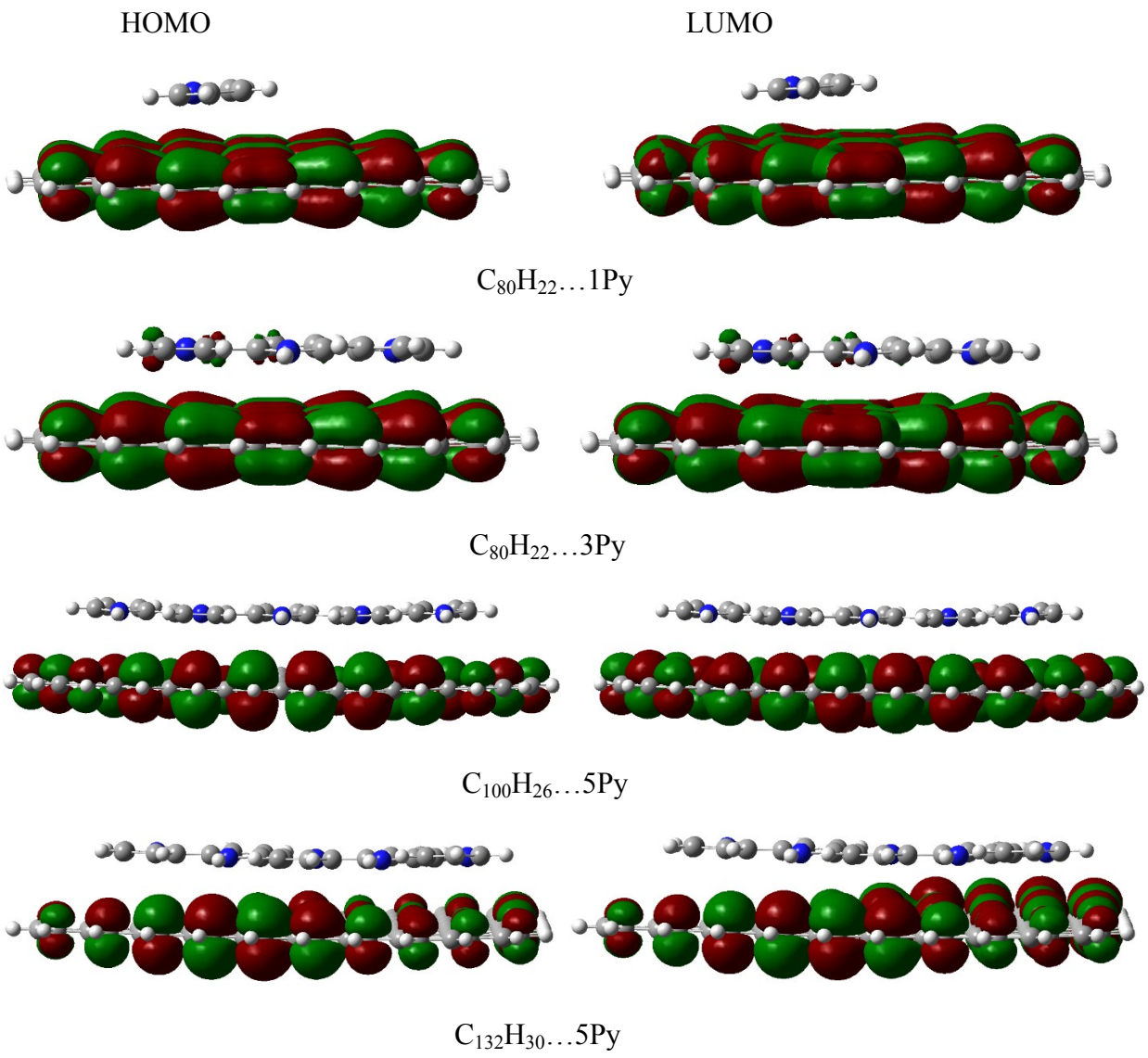


Figure S8. HOMO-LUMO orbitals of π stacked orientation of $C_{80}H_{22}$…1Py, $C_{80}H_{22}$…3Py, $C_{100}H_{26}$…5Py and $C_{132}H_{30}$…5Py composites.

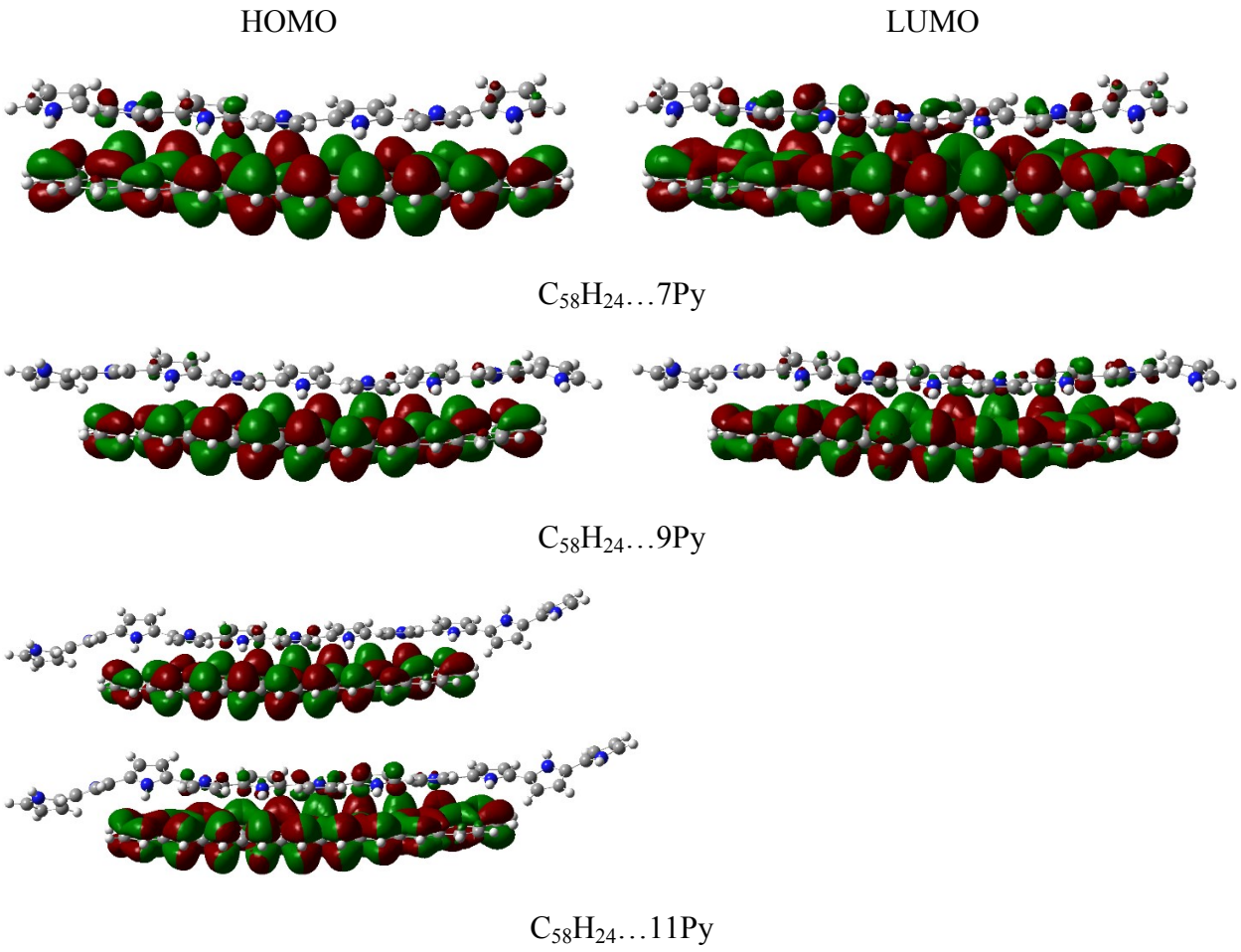


Figure S9. HOMO-LUMO orbitals of π stacked orientation of $C_{58}H_{24}$…nPy composites.

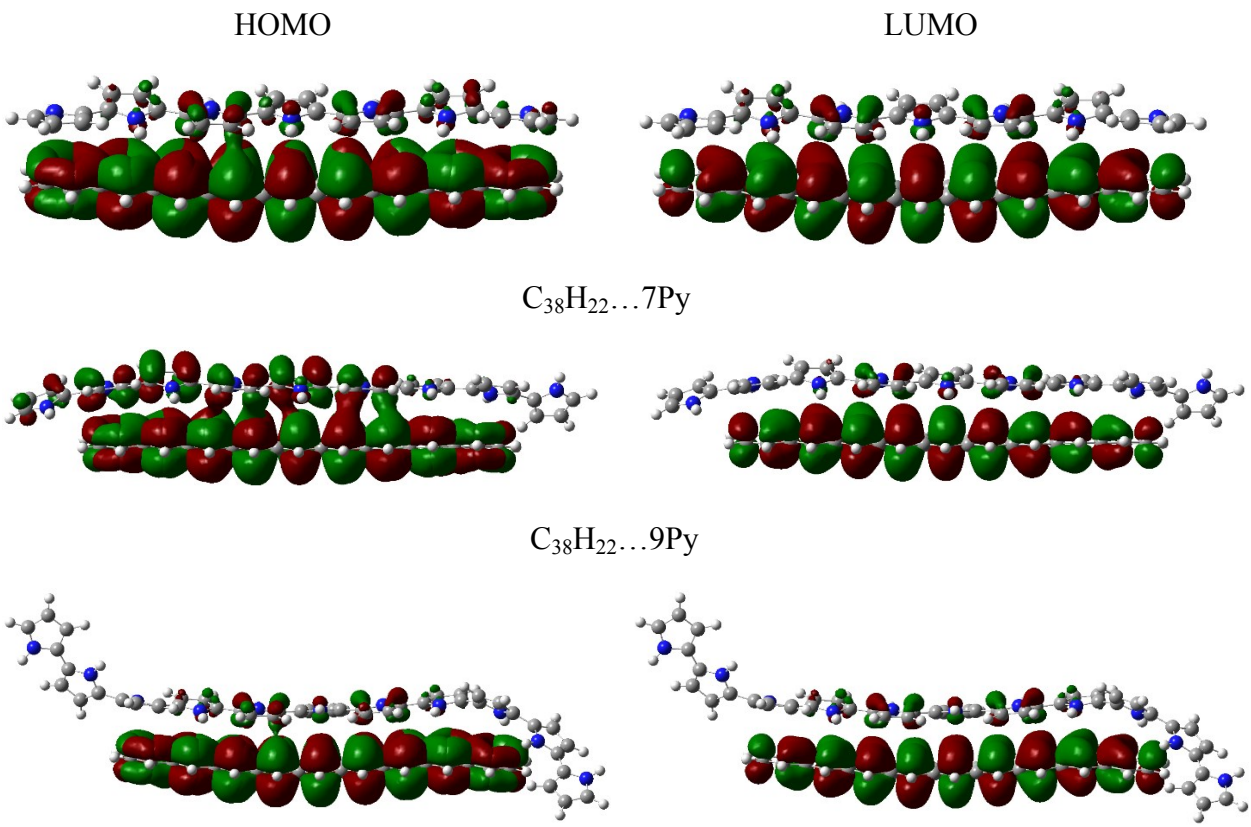


Figure S10. HOMO-LUMO orbitals of $C_{38}H_{22}$…nPy composites.