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

Interaction of Nucleobases with Silicon Doped and Defective Silicon Doped Graphene and Optical properties

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Table S1 The Interaction energies (IEs) (kcal/mol) for the 5SiGr-NBs Complexes in the Presence and Absence of Electric Field

Model	Z(+)	Z(-)	Absence
5SiGr-A	-53.55	-56.63	-55.06
5SiGr-G	-60.25	-58.26	-57.34
5SiGr-T	-46.77	-48.80	-47.80
5SiGr-C	-56.52	-62.29	-61.30
5SiGr-U	-42.76	-44.85	-43.90

Table S2 The Energy Decomposition Analysis of the Complexes formed by NBs with Gr-L, SiGr-L, 5SiGr-L and 57SiGr-L

Model	NB	Ele. Stat Energy (kcal/mol)	Pau. Rep Energy (kcal/mol)	Orb. Int Energy (kcal/mol)	Disp. Energy (kcal/mol)	Inter. Energy (kcal/mol)
Gr-L	A	-11.78	30.96	-6.47	-32.74	-20.04
	G	-13.04	34.87	-9.61	-35.84	-23.62
	T	-10.95	30.28	-7.21	-31.40	-19.28
	C	-10.78	28.52	-7.72	-28.53	-18.50
	U	-9.67	26.36	-6.43	-26.95	-16.69
SiGr-L	A	-140.74	227.36	-102.10	-16.32	-31.80
	G	-134.88	239.72	-115.42	-35.35	-45.92
	T	-115.65	203.21	-91.18	-27.79	-31.41
	C	-138.94	239.67	-117.09	-27.05	-43.41
	U	-126.42	211.74	-99.20	-13.55	-27.43
5SiGr-L	A	-111.93	165.22	-86.15	-21.90	-54.78
	G	-95.01	167.33	-92.34	-40.25	-60.27
	T	-87.79	152.02	-75.87	-34.01	-45.65
	C	-99.66	166.06	-93.48	-30.67	-57.75
	U	-84.36	144.57	-73.88	-27.76	-41.42
57SiGr-L	A	-132.58	212.07	-98.54	-19.53	-38.58
	G	-124.51	219.66	-108.94	-35.58	-49.37
	T	-118.00	205.99	-96.71	-34.65	-43.36
	C	-127.59	222.40	-114.36	-29.55	-49.10
	U	-108.01	186.41	-85.82	-24.89	-32.32

Ele. Stat Energy = Electrostatic Energy, Orb. Int Energy = Orbital Interaction Energy, Pau. Rep Energy = Pauli Repulsion Energy, Disp. Energy = Dispersion Energy, Inter. Energy = Interaction Energy.

Table S3 The Second-Order Perturbation Theory Analysis of Fock Matrix for the Complex Formed by SiGr-L, 5SiGr-L and 57SiGr-L with NBs

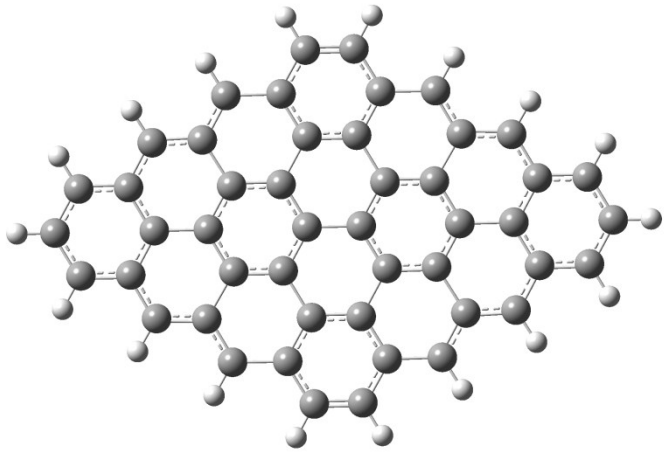
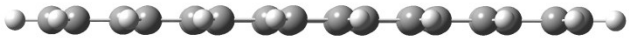
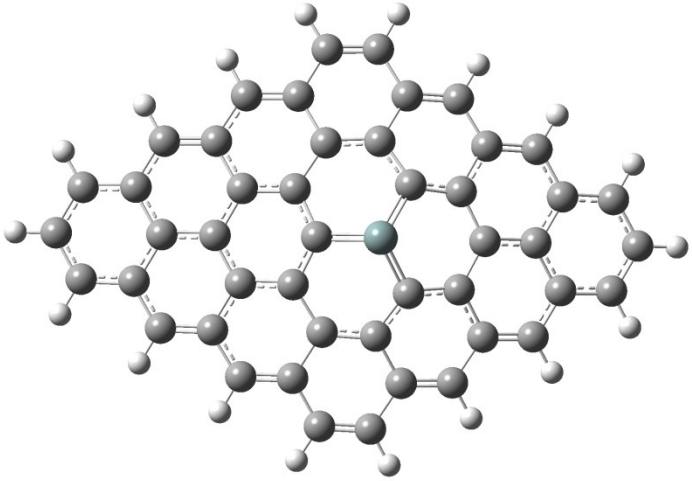
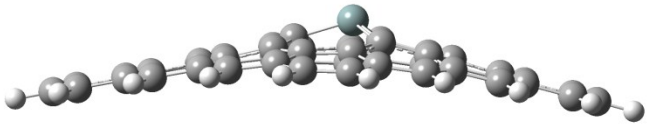
Complex	Charge Transfer Interaction	$E^{(2)}$ (kcal/mol)
SiGr-L-A	LP (N) ⟶ LP* (Si)	154.28
SiGr-L-G	LP (O) ⟶ LP* (Si)	215.72
SiGr-L-T	LP (O) ⟶ LP* (Si)	199.11
SiGr-L-C	LP (O) ⟶ LP* (Si)	243.77
SiGr-L-U	LP (O) ⟶ LP* (Si)	170.26
5SiGr-L-A	LP (N) ⟶ LP* (Si)	220.99
5SiGr-L-G	LP (O) ⟶ LP* (Si)	267.29
5SiGr-L-T	LP (O) ⟶ LP* (Si)	245.95
5SiGr-L-C	LP (O) ⟶ LP* (Si)	278.27
5SiGr-L-U	LP (O) ⟶ LP* (Si)	243.16
57SiGr-L-A	LP (N) ⟶ LP* (Si)	154.76
57SiGr-L-G	LP (O) ⟶ LP* (Si)	207.64
57SiGr-L-T	LP (O) ⟶ LP* (Si)	183.60
57SiGr-L-C	LP (O) ⟶ LP* (Si)	230.15
57SiGr-L-U	LP (O) ⟶ LP* (Si)	175.59

LP is lone pair occupied orbital and LP* is unoccupied orbital

Table S4 The Calculated NICS (0) values at the Center of Pyrimidine and Imidazole Ring of Nucleobases (A, G, T, C and U)

Model	G		A		T	C	U
	Pyr	Imi	Pyr	Imi	Pyr	Pyr	Pyr
Parent	-3.13	-12.82	-7.07	-9.57	-1.45	-1.30	-1.27
Gr-L	-11.26	-20.60	-15.02	-19.95	-9.84	-9.51	-9.36
SiGr-L	-11.87	-16.93	-9.49	-14.81	-7.26	-9.19	-5.16
5SiGr-L	-16.81	-21.20	-15.01	-20.10	-12.02	-13.96	-11.38
57SiGr-L	-8.76	-14.99	-7.91	-14.36	-6.37	-6.73	-4.15

Pyr - pyrimidine ring, Imi – imidazole ring

Top View	Side View
 Gr	
 SiGr	

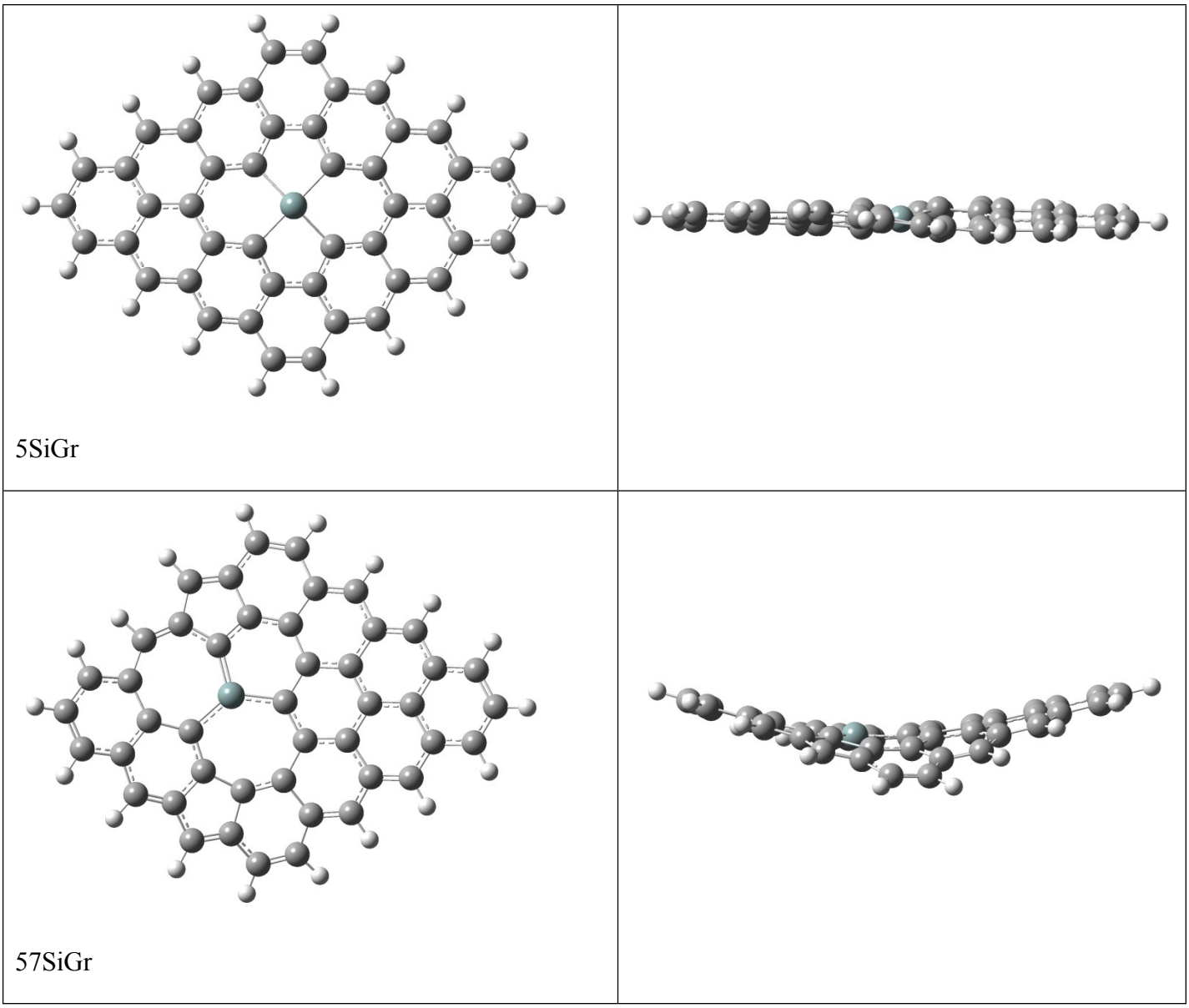
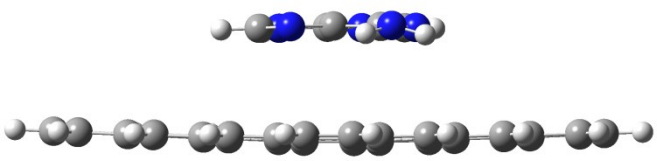
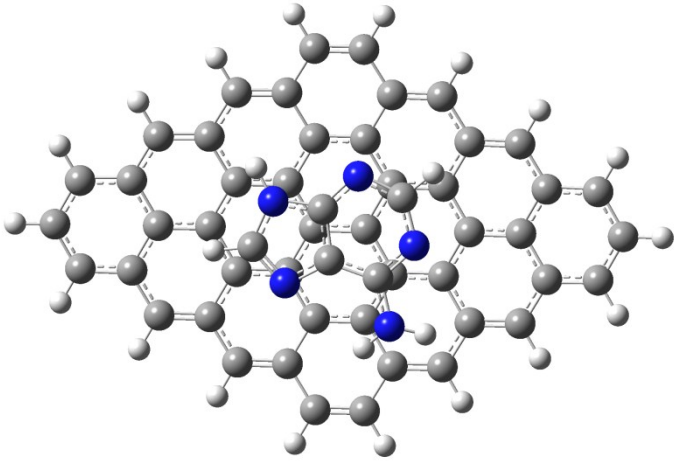
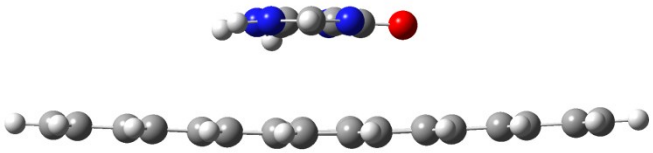
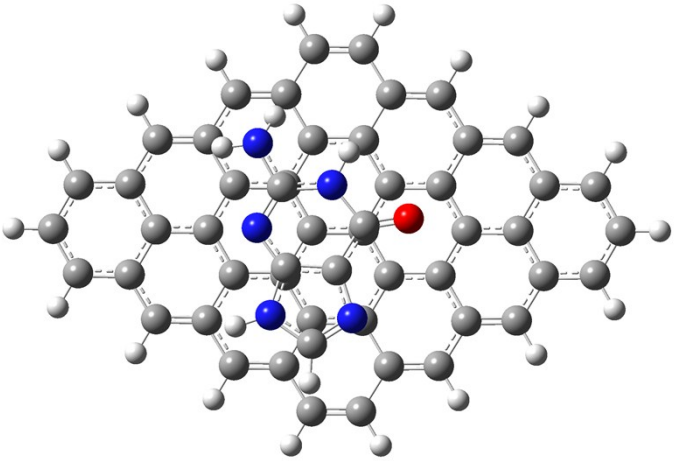
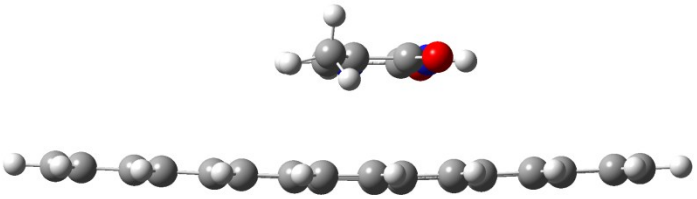
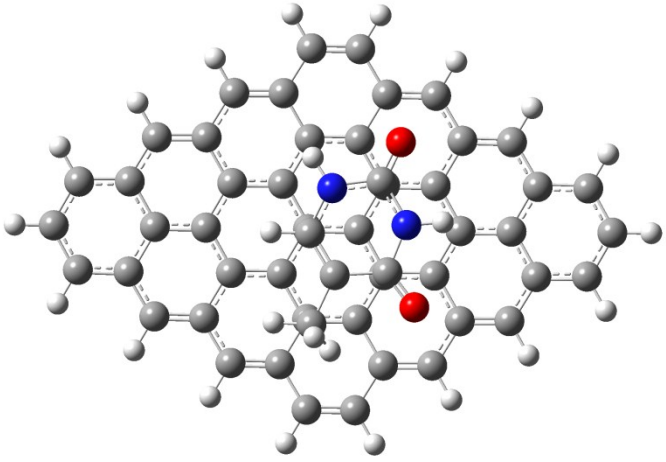
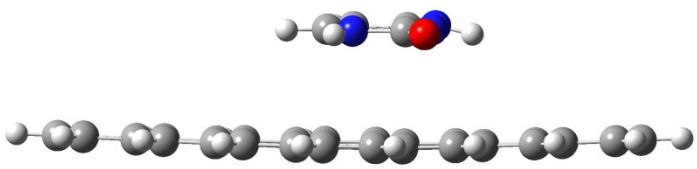
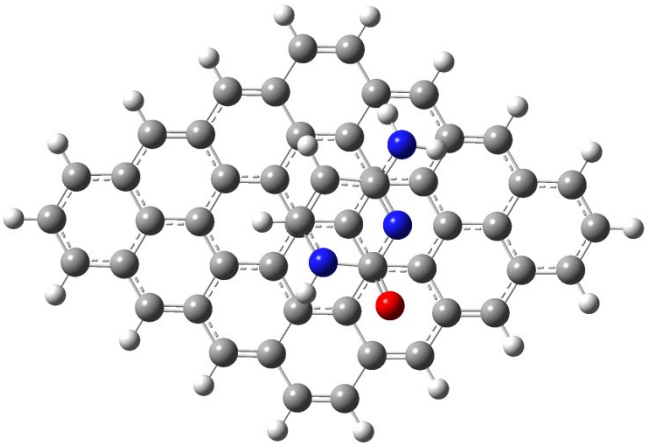
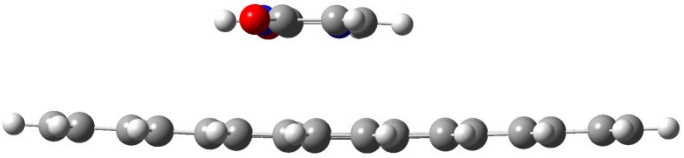
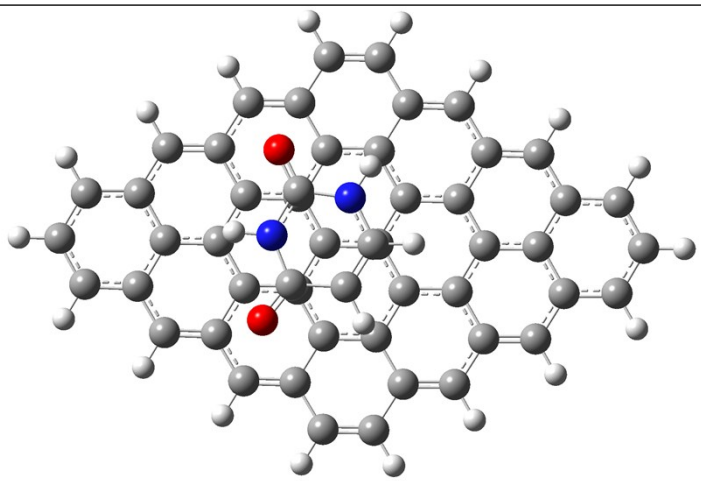
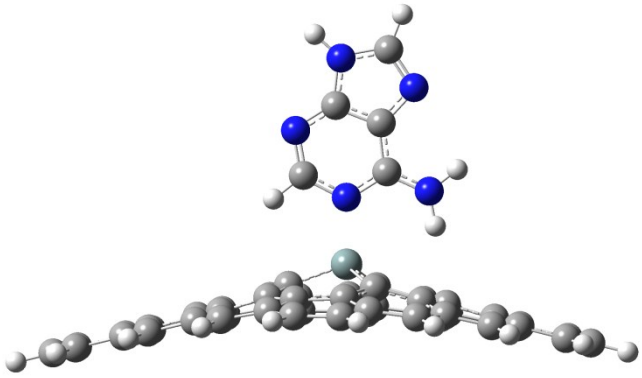
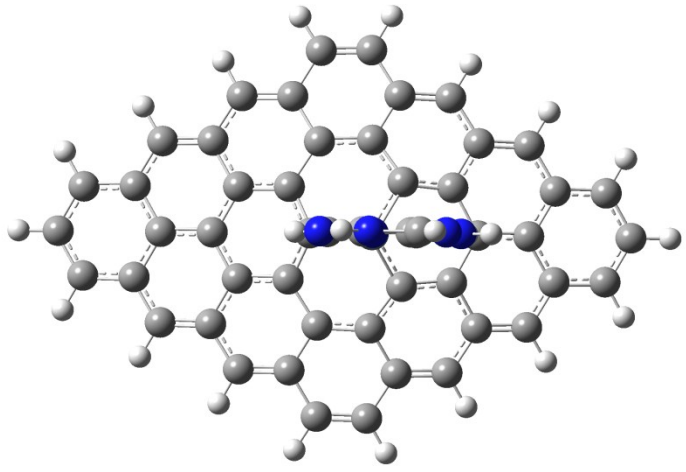
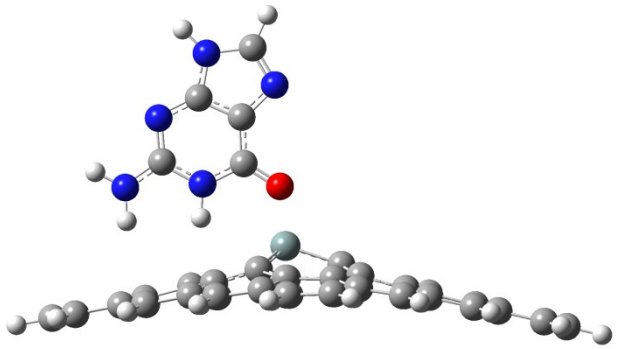
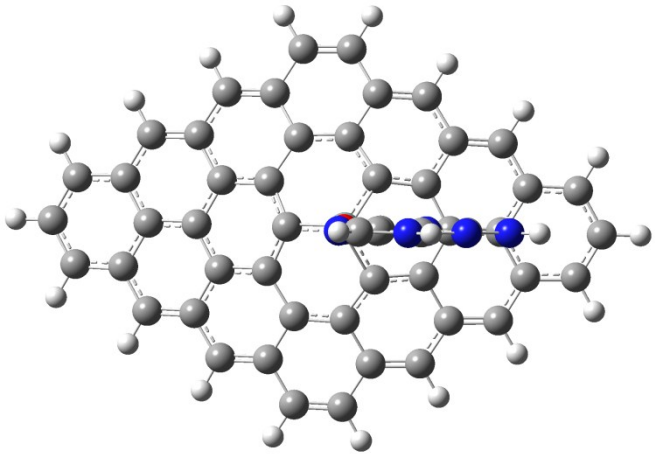
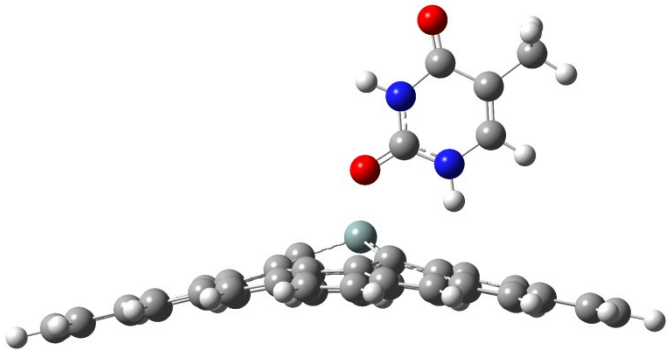
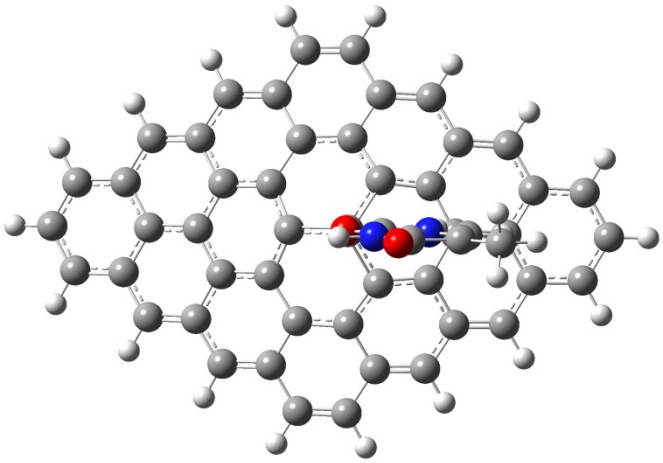
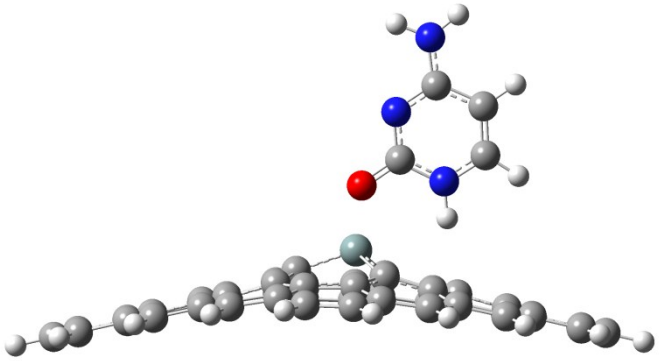
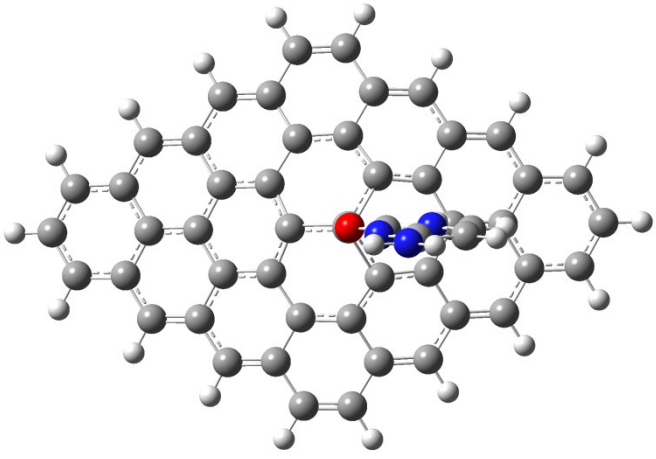
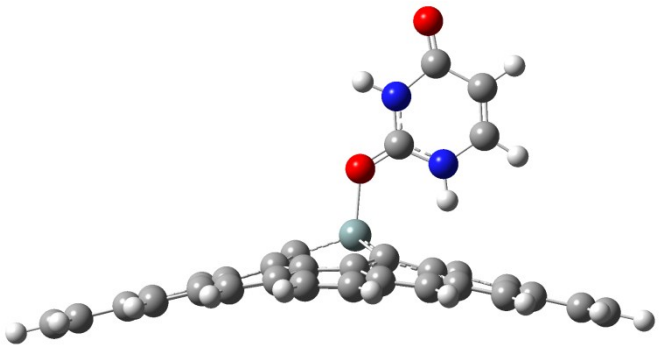
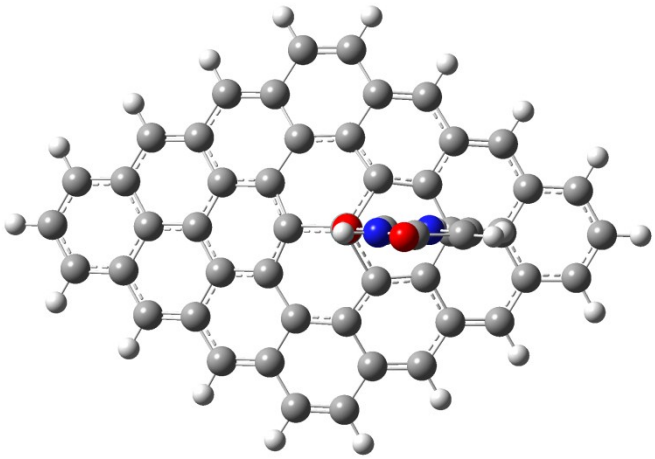
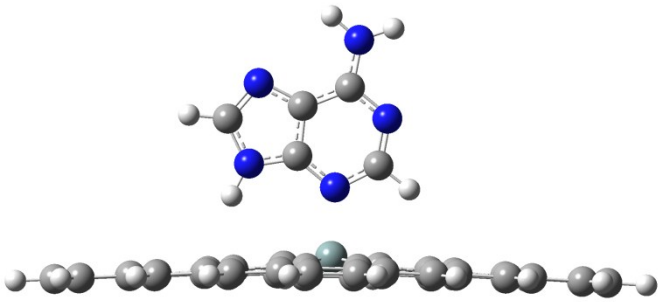
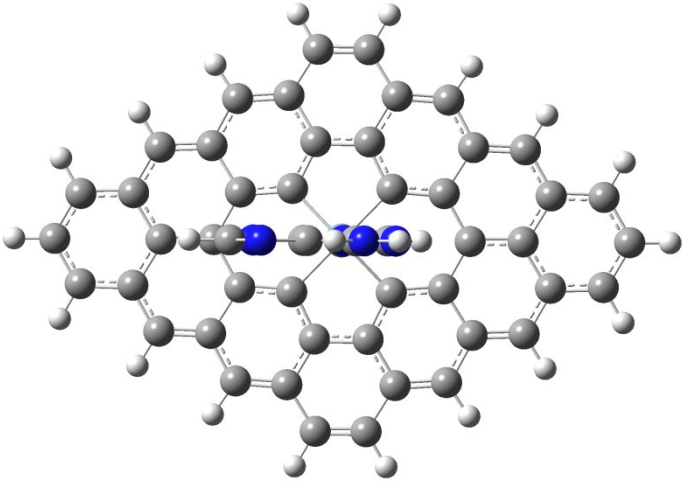
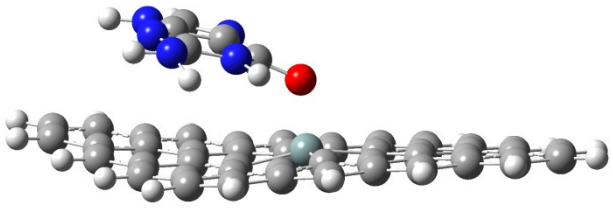
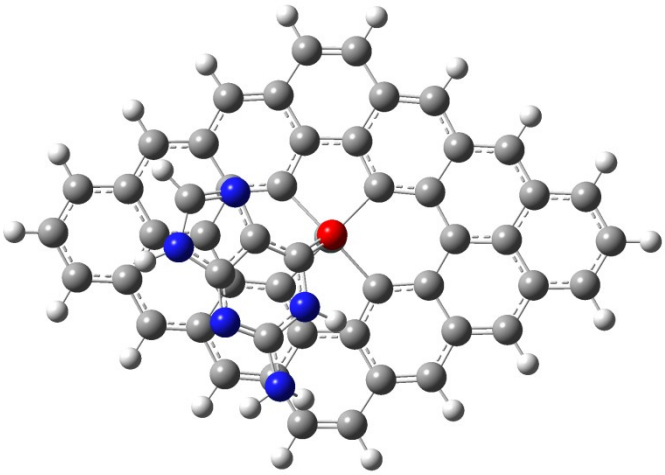


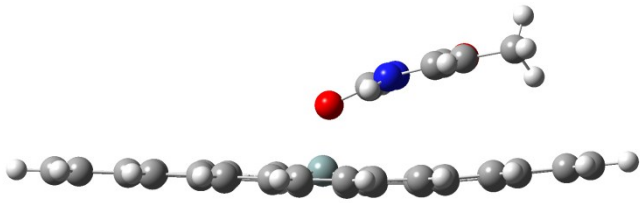
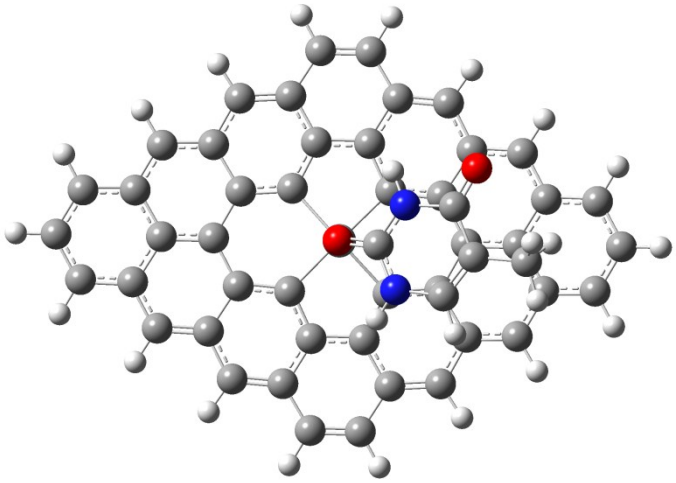
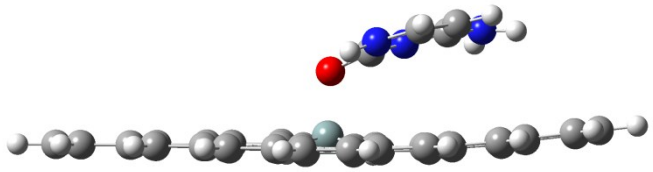
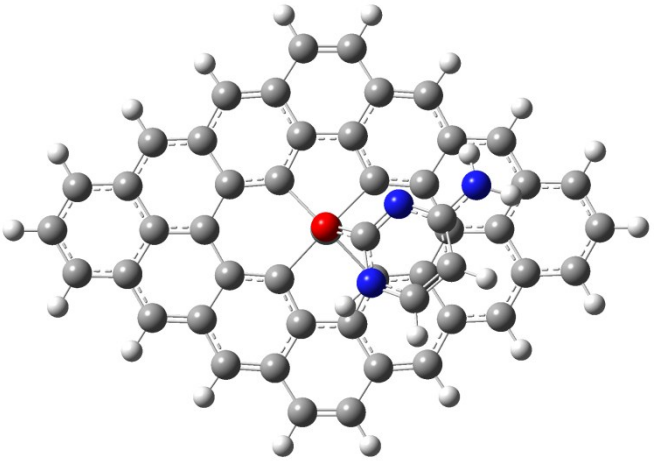
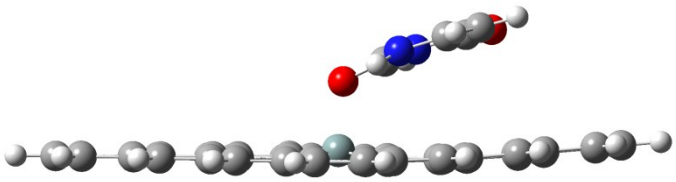
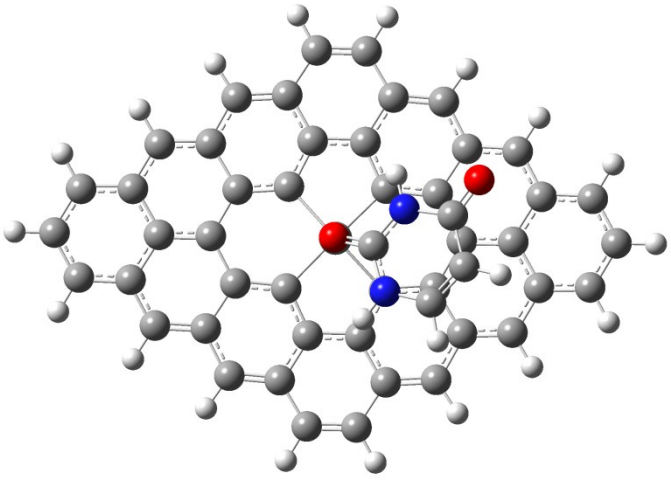
Fig. S1 The optimized geometries of Gr, SiGr, 5SiGr and 57SiGr at M06-2X/6-31+G** level of theory.

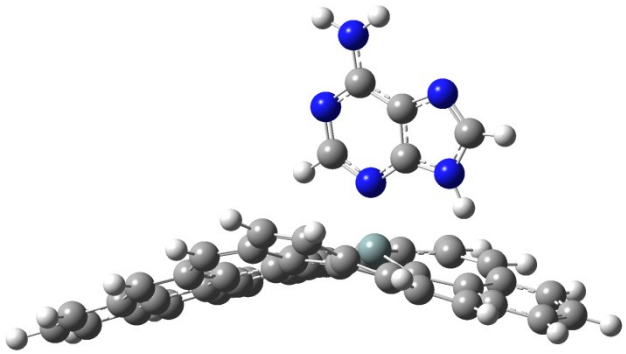
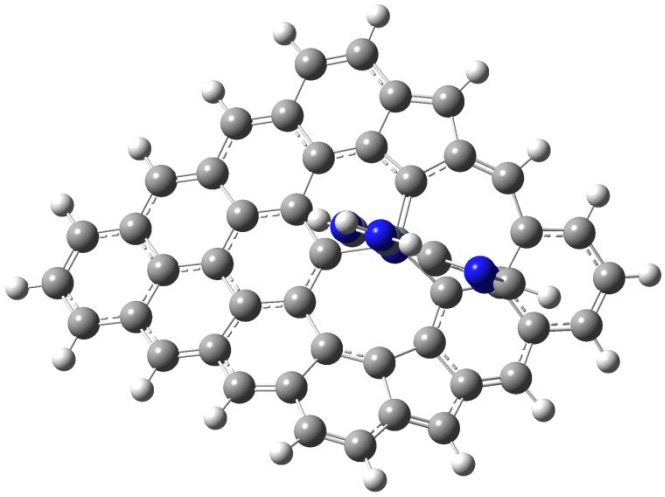
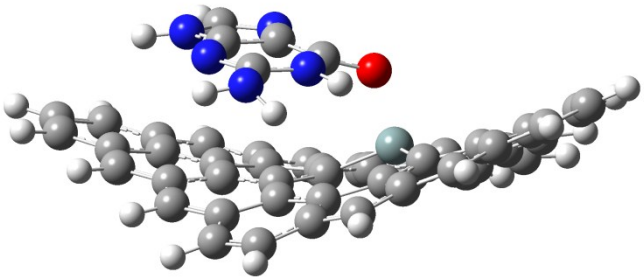
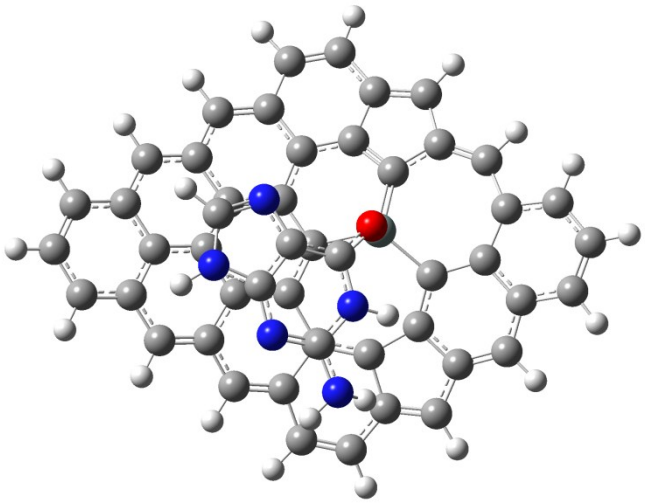
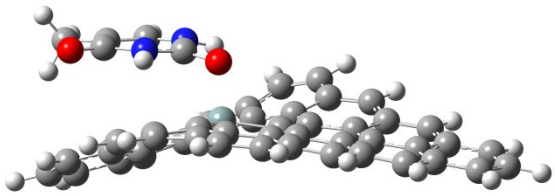
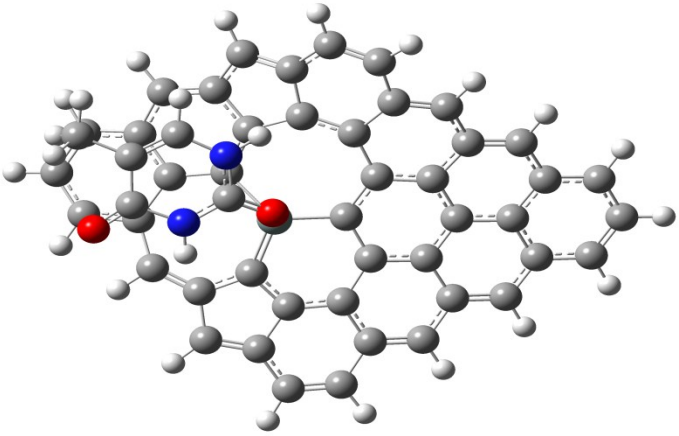
Side View	Top View
 Gr-A	
 Gr-G	
 Gr-T	

 Gr-C	
 Gr-U	
 SiGr-A	

 SiGr-G	
 SiGr-T	
 SiGr-C	

 SiGr-U	
 5SiGr-A	
 5SiGr-G	

 5SiGr-T	
 5SiGr-C	
 5SiGr-U	

 57SiGr-A	
 57SiGr-G	
 57SiGr-T	

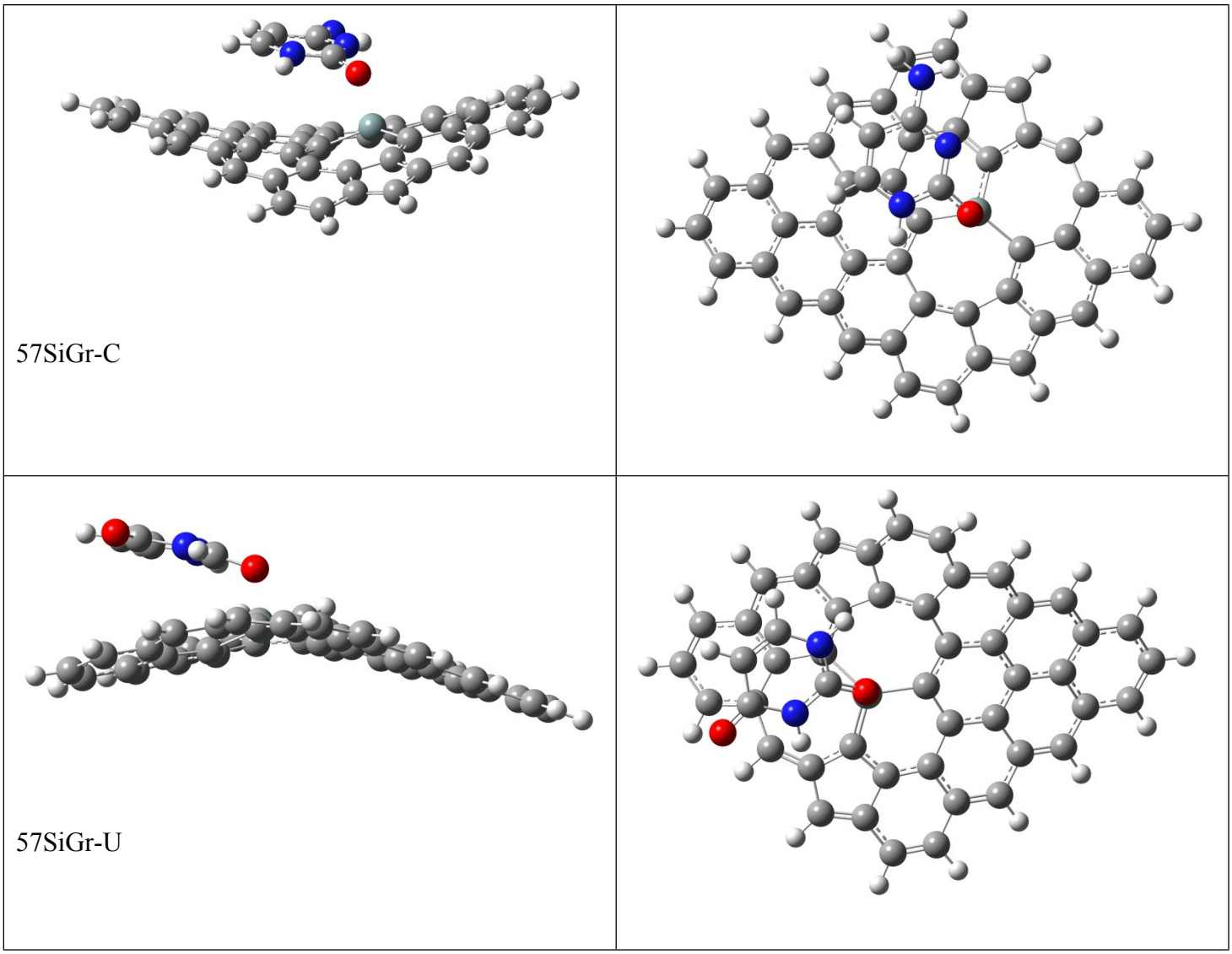
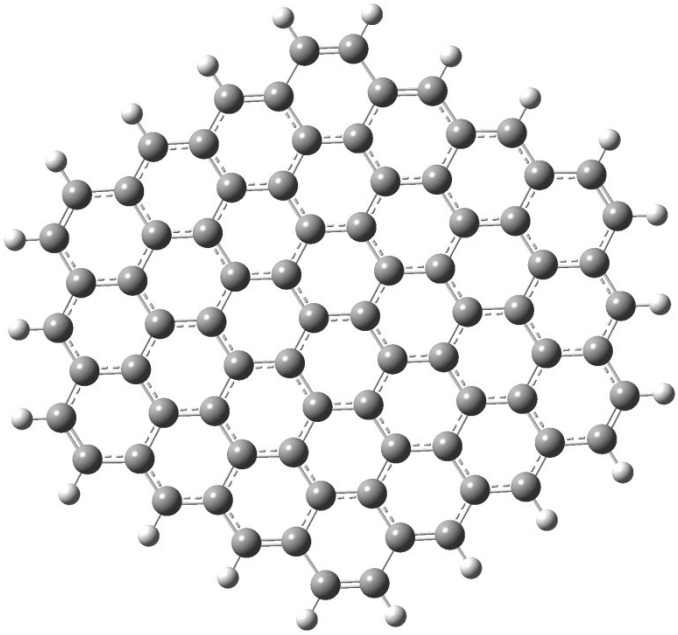
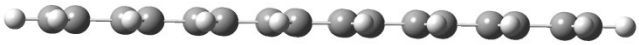
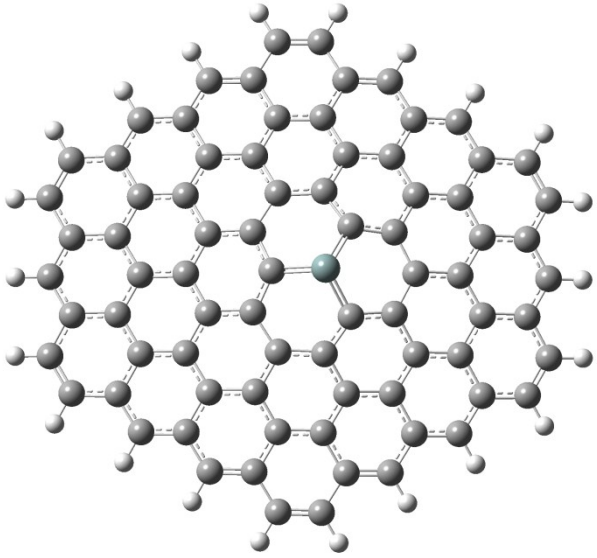
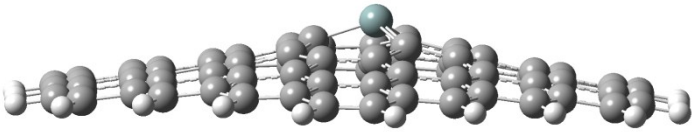
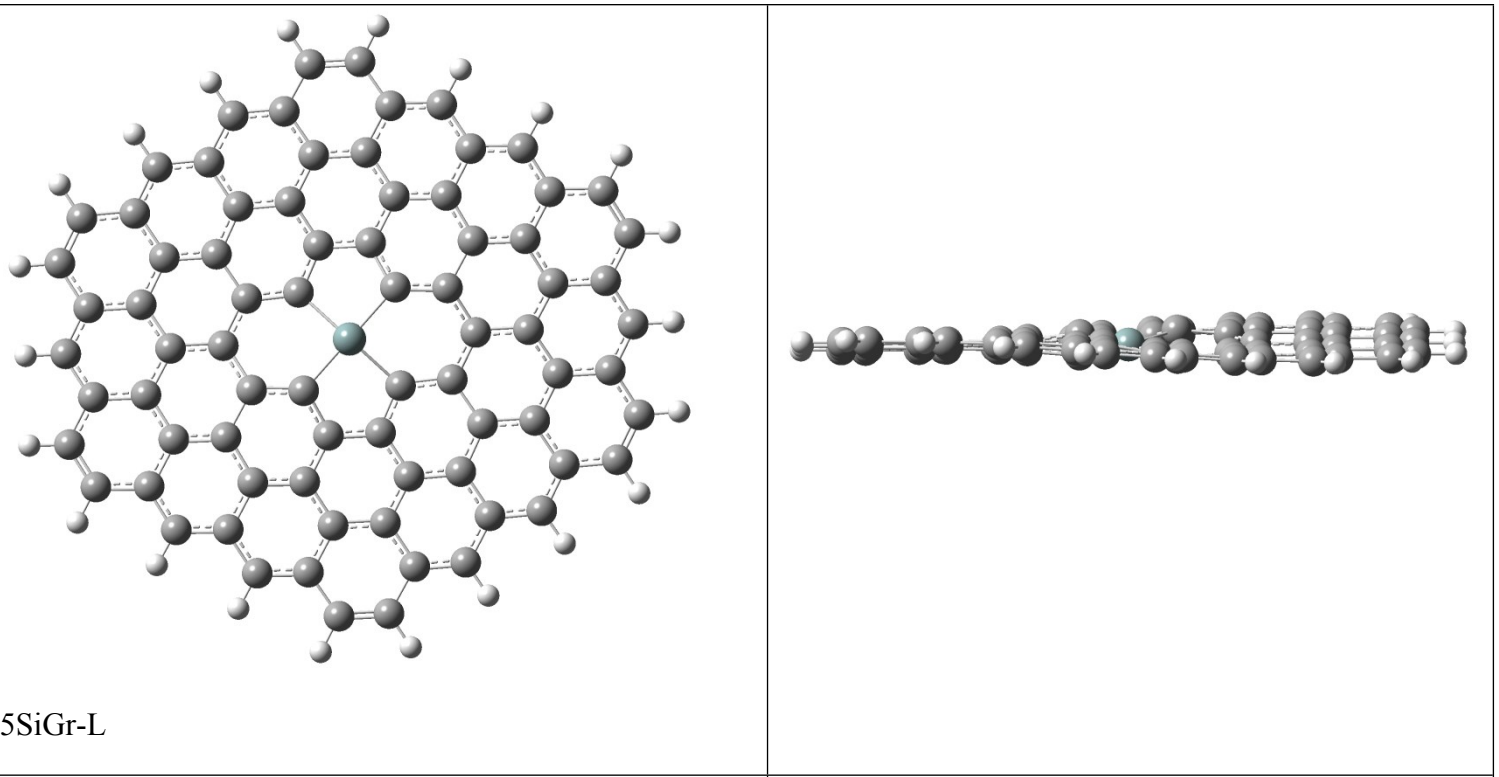
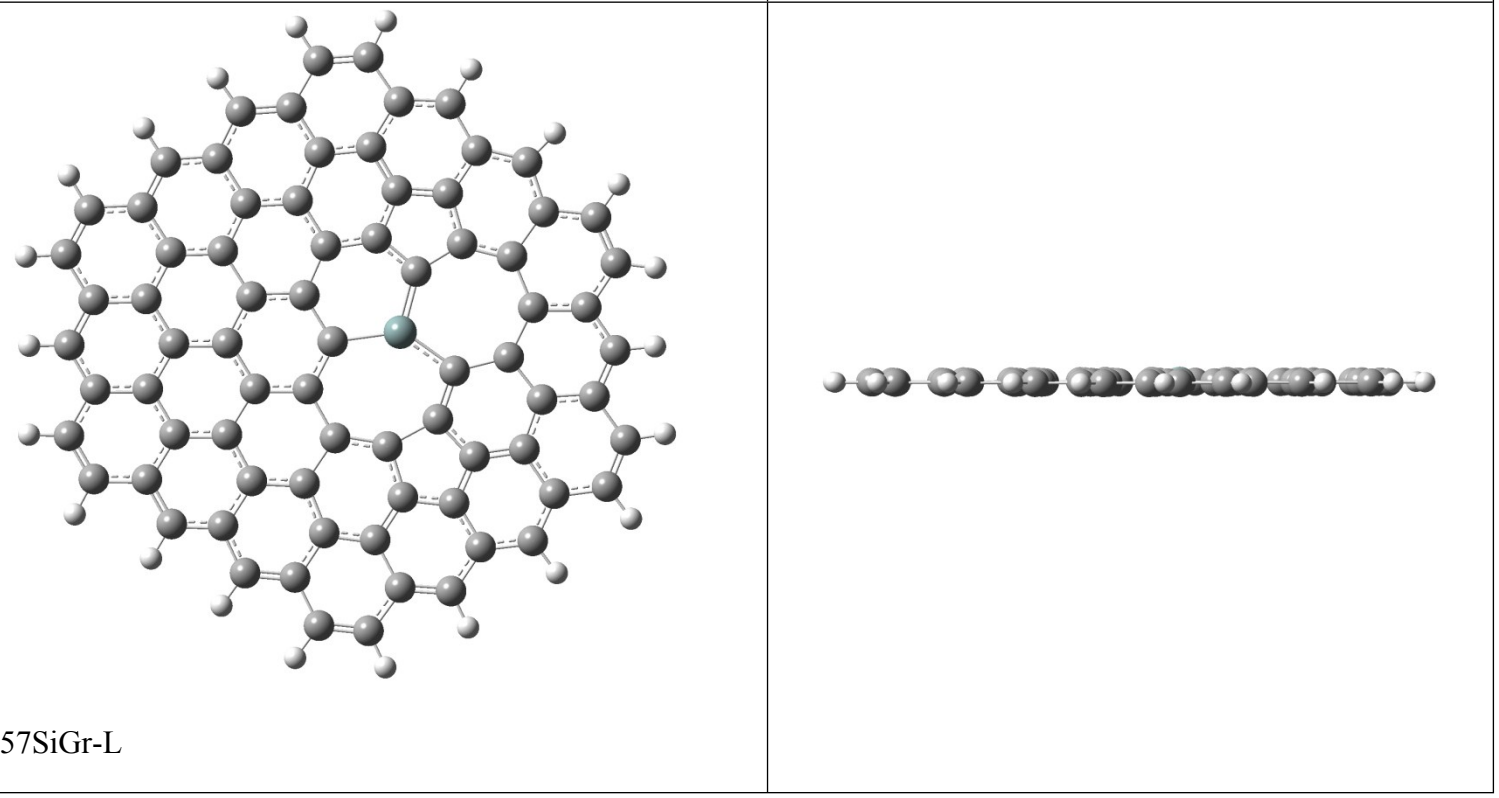


Fig. S2 The optimized geometries of the complexes of Gr, SiGr, 5SiGr and 57SiGr with NBs at M062X/6-31+G** level of theory.

Top View	Side View
 Gr-L	
 SiGr-L	

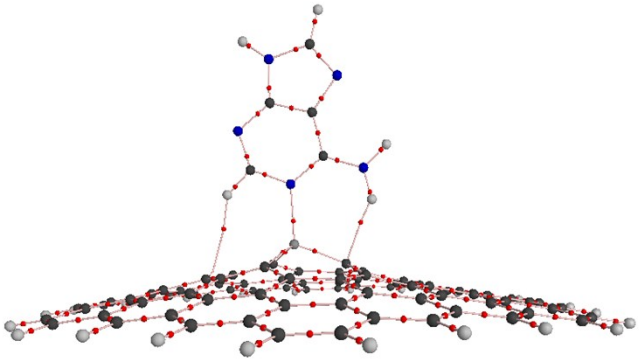


5SiGr-L

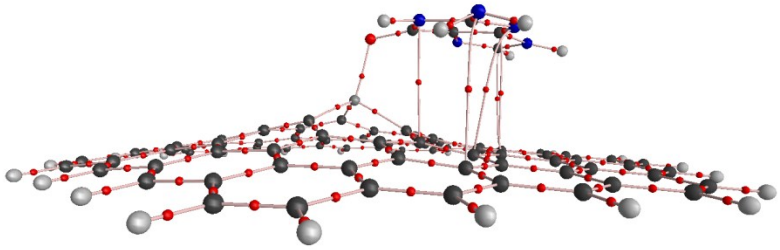


57SiGr-L

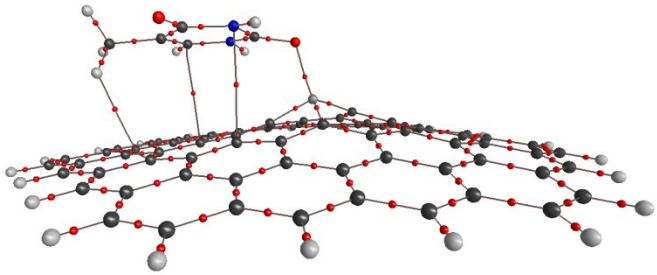
Fig. S3 The optimized geometries of Gr-L, SiGr-L, 5SiGr-L and 57SiGr-L at M06-2X/6-31+G** level of theory.



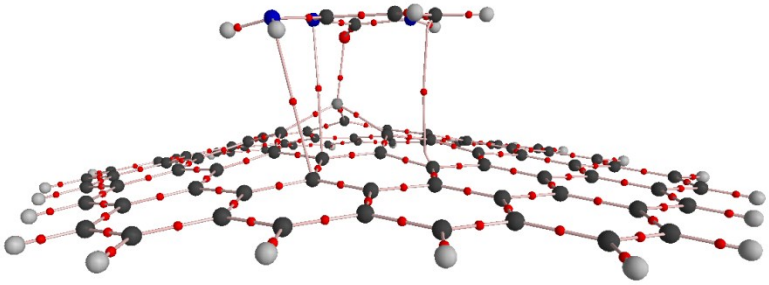
SiGr-L-A



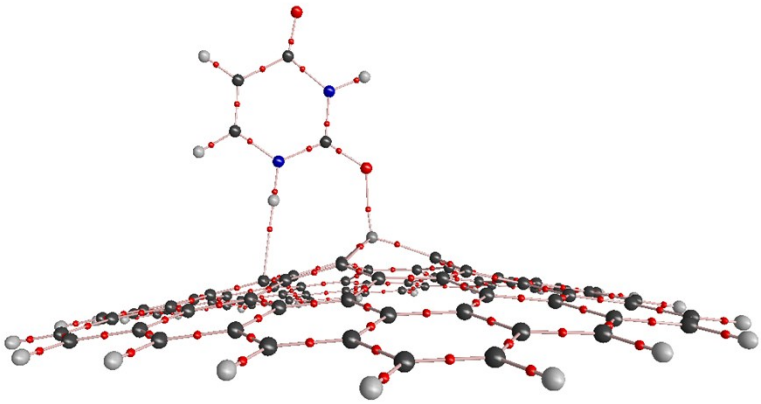
SiGr-L-G



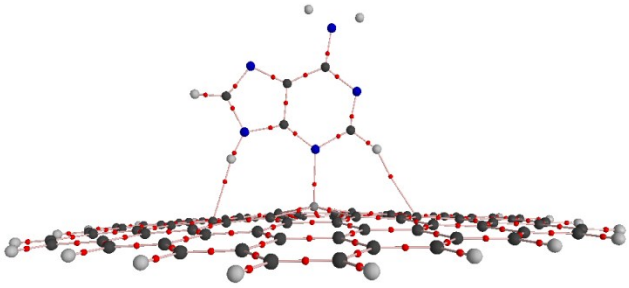
SiGr-L-T



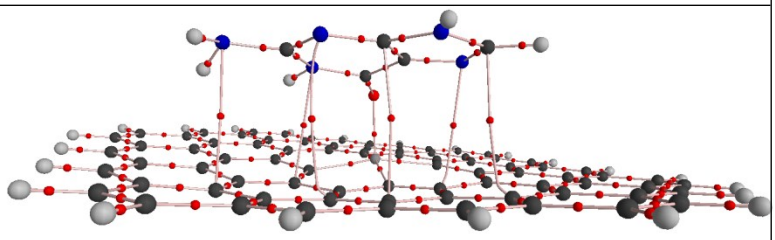
SiGr-L-C



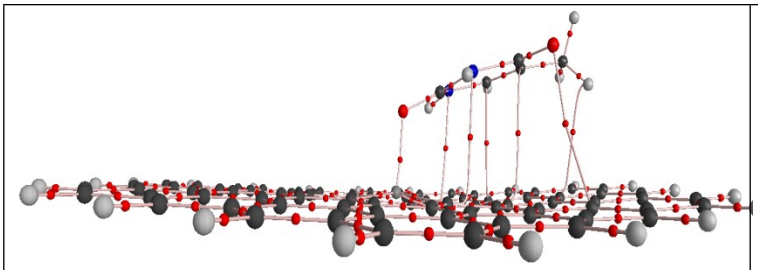
SiGr-L-U



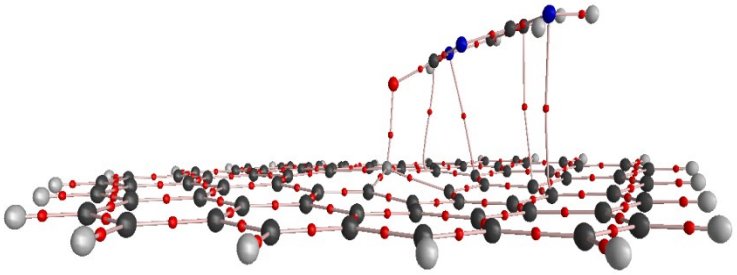
5SiGr-L-A



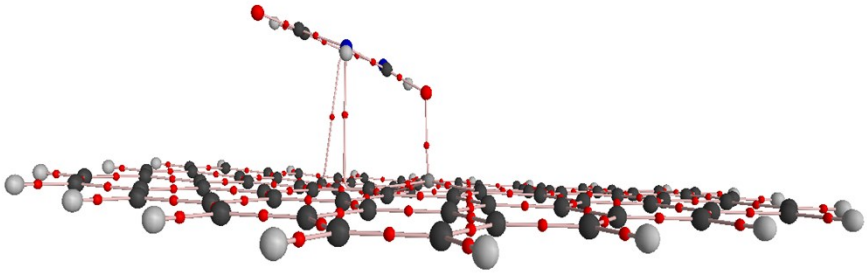
5SiGr-L-G



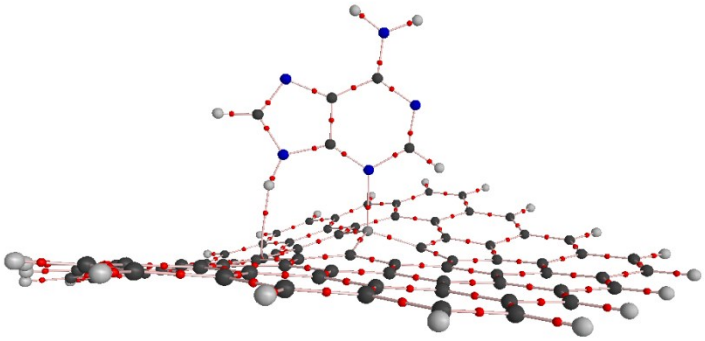
5SiGr-L-T



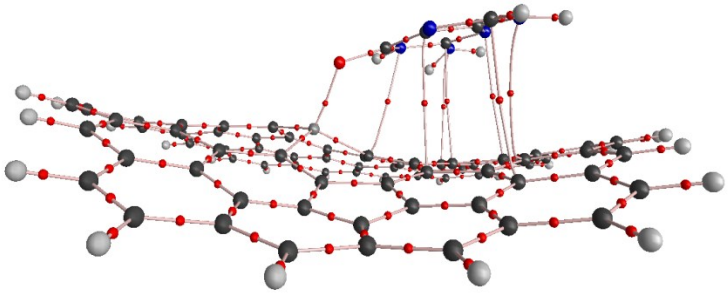
5SiGr-L-C



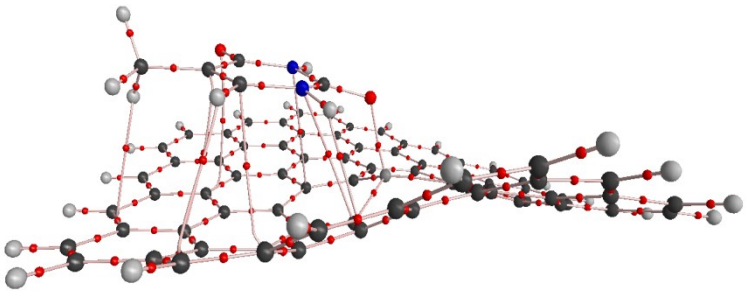
5SiGr-L-U



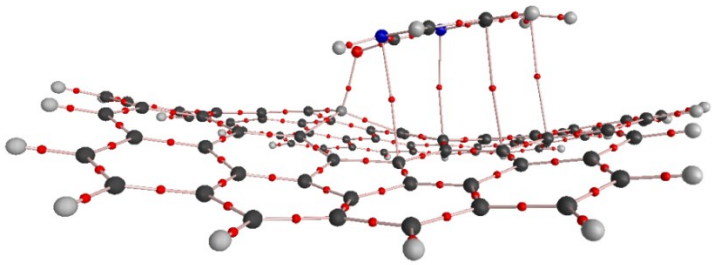
57SiGr-L-A



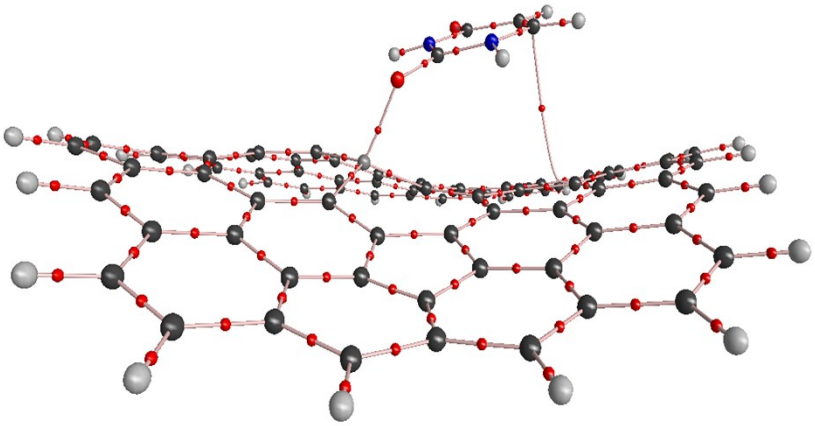
57SiGr-L-G



57SiGr-L-T

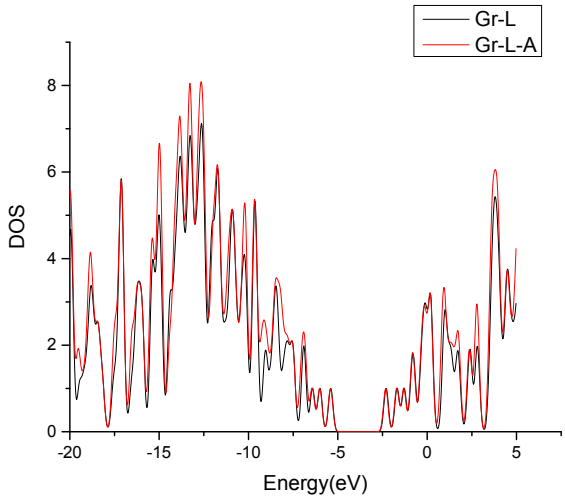


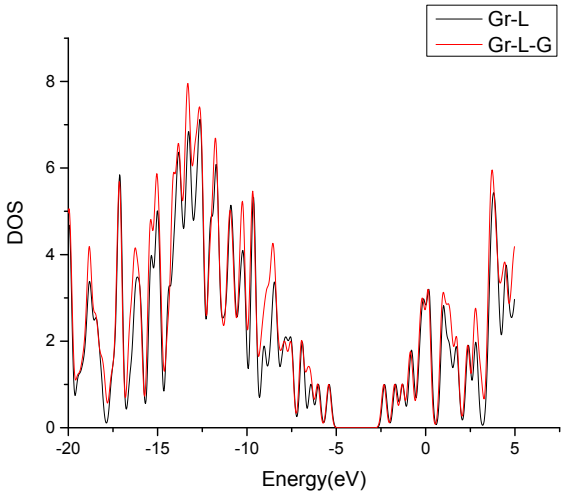
57SiGr-L-C

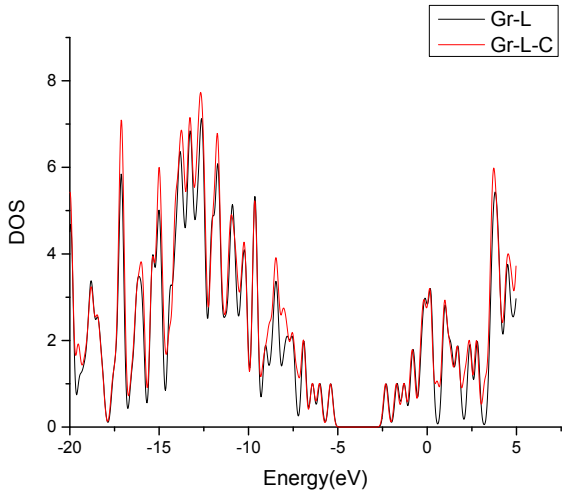


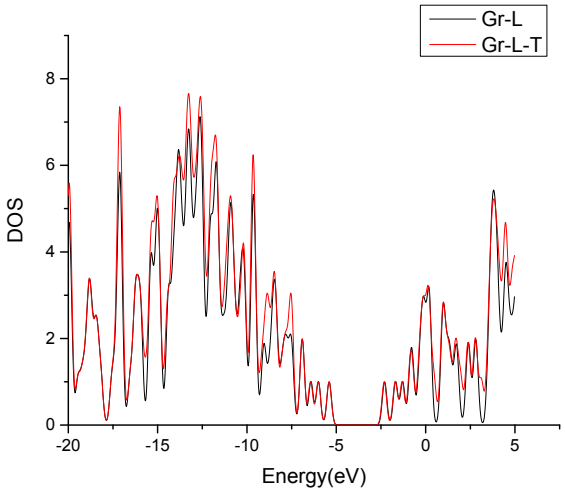
57SiGr-U

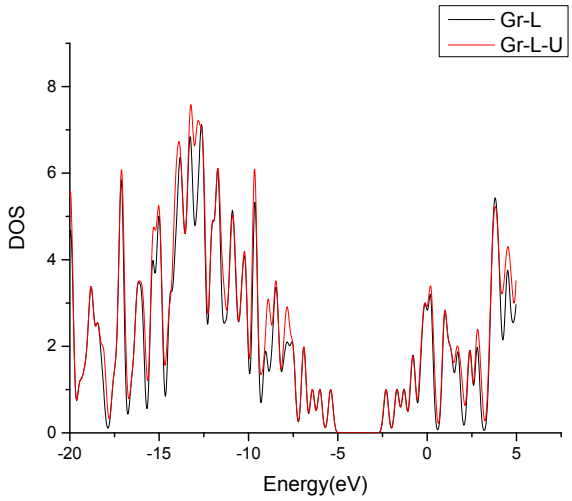
Fig. S4 The molecular graphs for the complexes of SiGr, 5SiGr and 57SiGr with NBs.

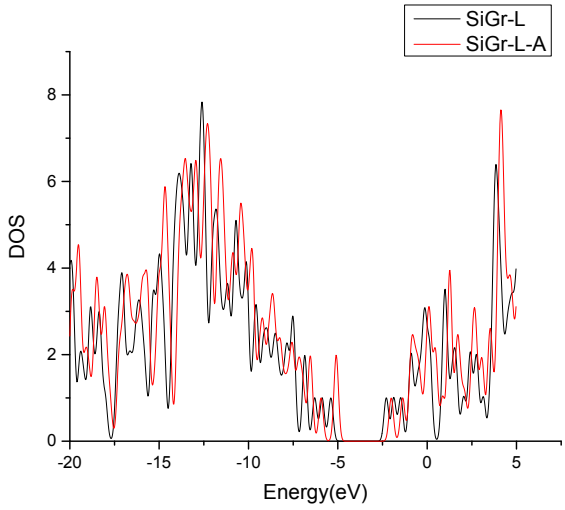

Gr-L
Gr-L-A
DOS
Energy(eV)

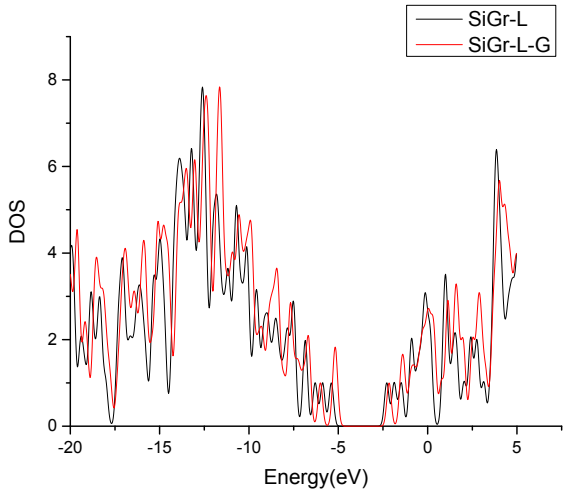

Gr-L
Gr-L-G
DOS
Energy(eV)

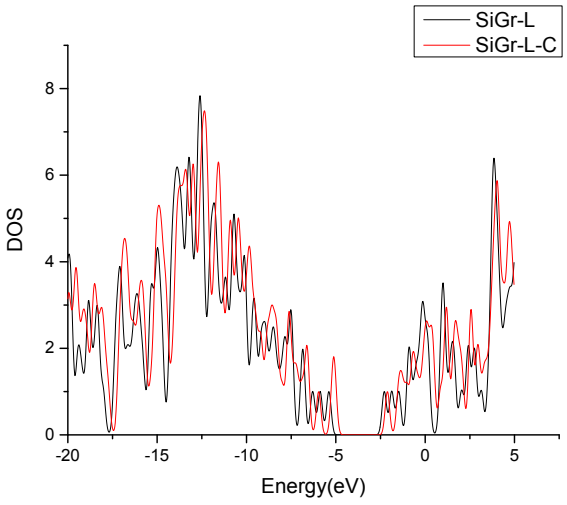

Gr-L
Gr-L-C
DOS
Energy(eV)

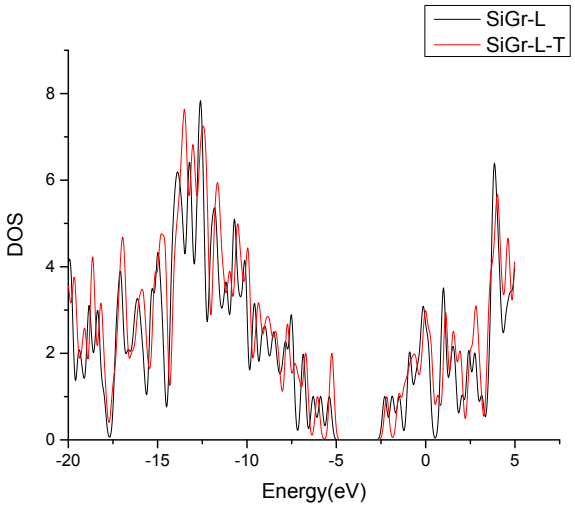

Gr-L
Gr-L-T
DOS
Energy(eV)

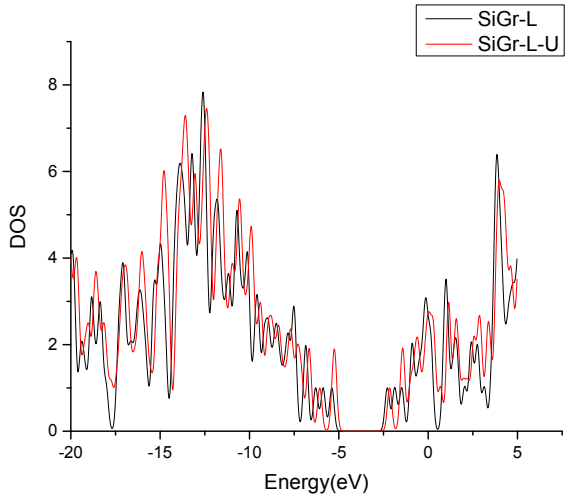

Gr-L
Gr-L-U
DOS
Energy(eV)

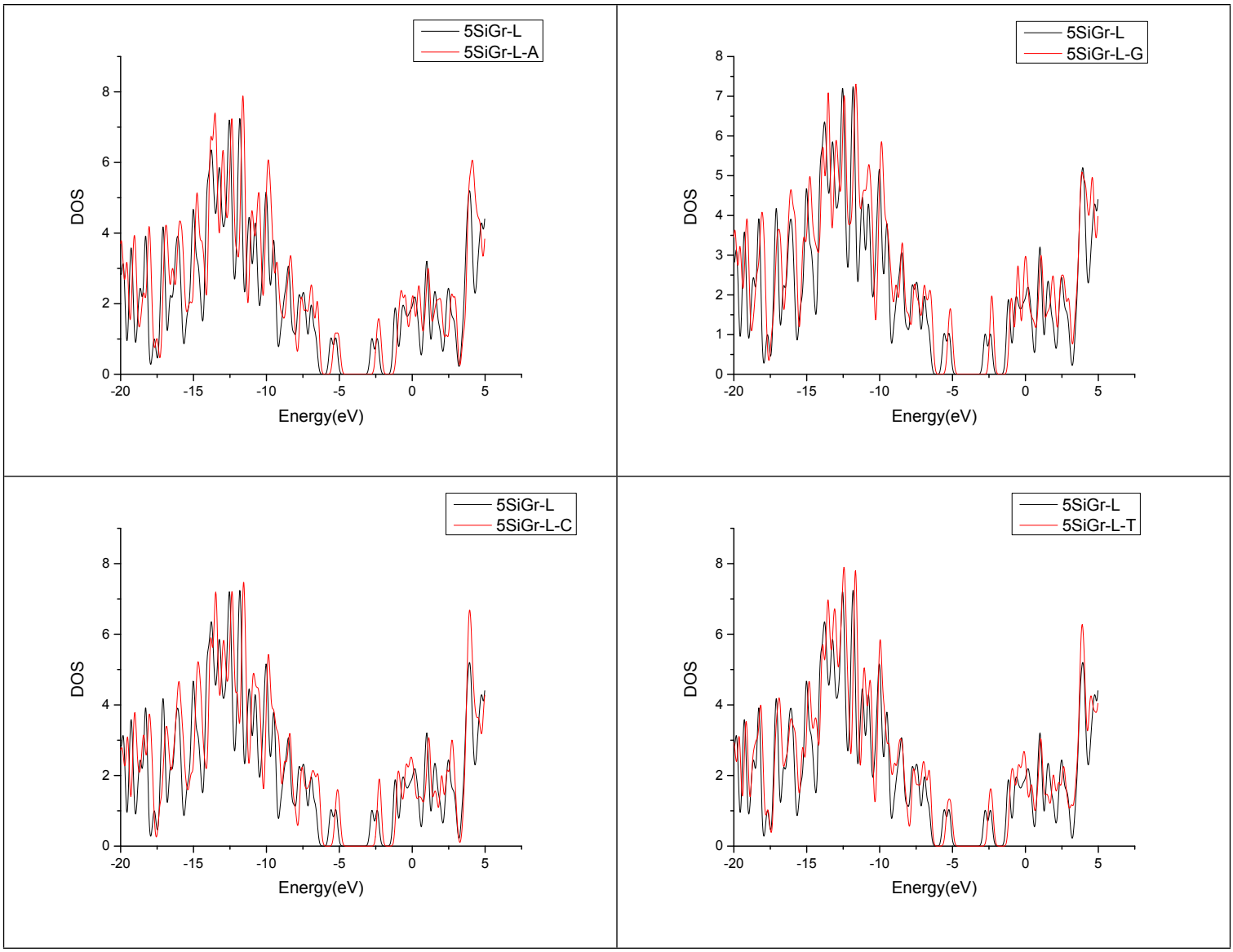

SiGr-L
SiGr-L-A
DOS
Energy(eV)

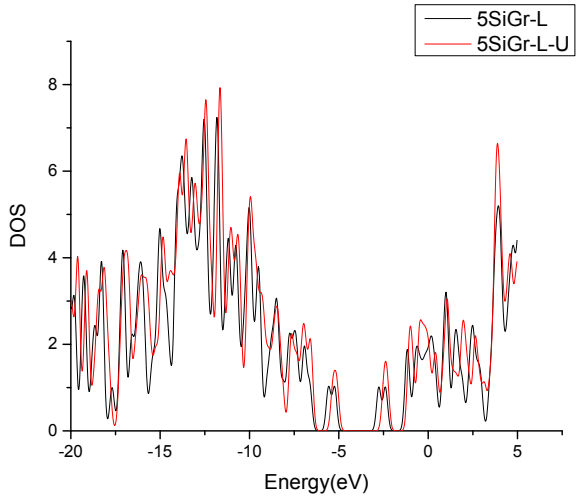

SiGr-L
SiGr-L-G
DOS
Energy(eV)

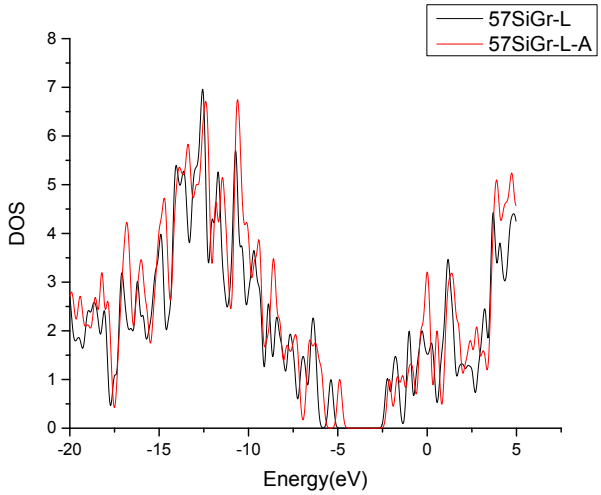

SiGr-L
SiGr-L-C
DOS
Energy(eV)

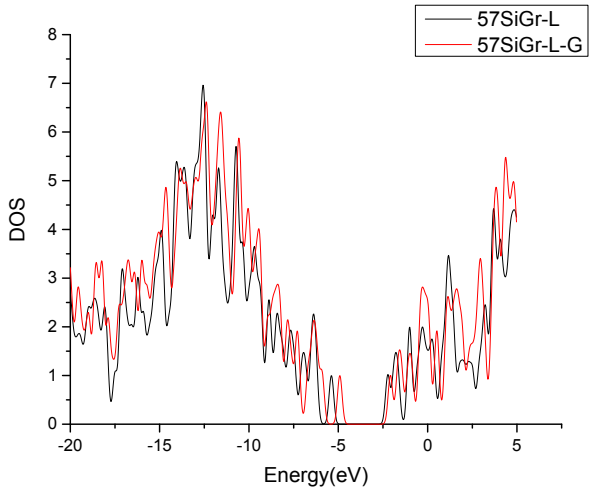

SiGr-L
SiGr-L-T
DOS
Energy(eV)


SiGr-L
SiGr-L-U
DOS
Energy(eV)


5SiGr-L
5SiGr-L-A
DOS
Energy(eV)
5SiGr-L
5SiGr-L-G
DOS
Energy(eV)
5SiGr-L
5SiGr-L-C
DOS
Energy(eV)
5SiGr-L
5SiGr-L-T
DOS
Energy(eV)


5SiGr-L
5SiGr-L-U
DOS
Energy(eV)


57SiGr-L
57SiGr-L-A
DOS
Energy(eV)


57SiGr-L
57SiGr-L-G
DOS
Energy(eV)

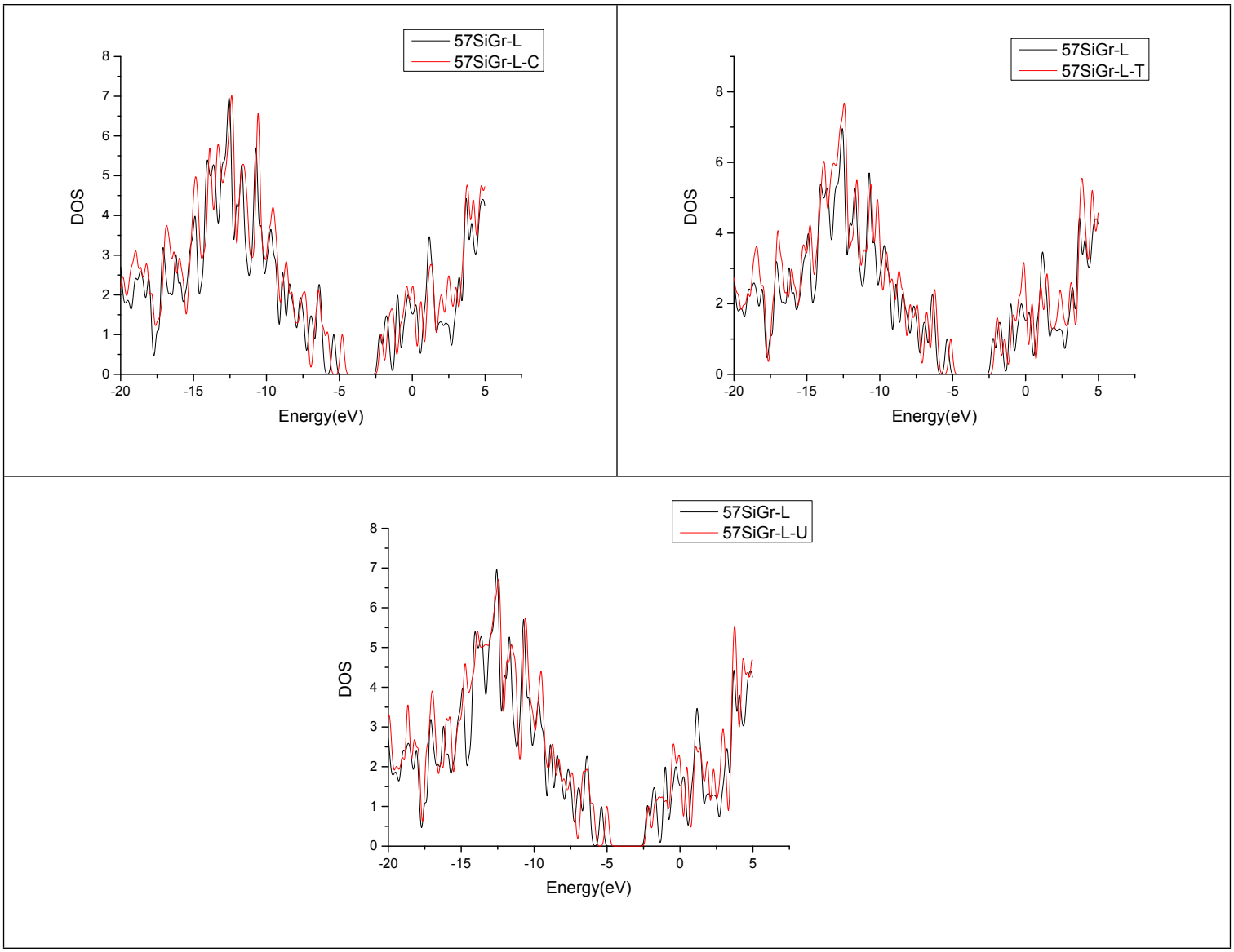


Fig. S5 The density of states (DOS) for all the complexes of Gr, SiGr, 5SiGr and 57SiGr with NBs.

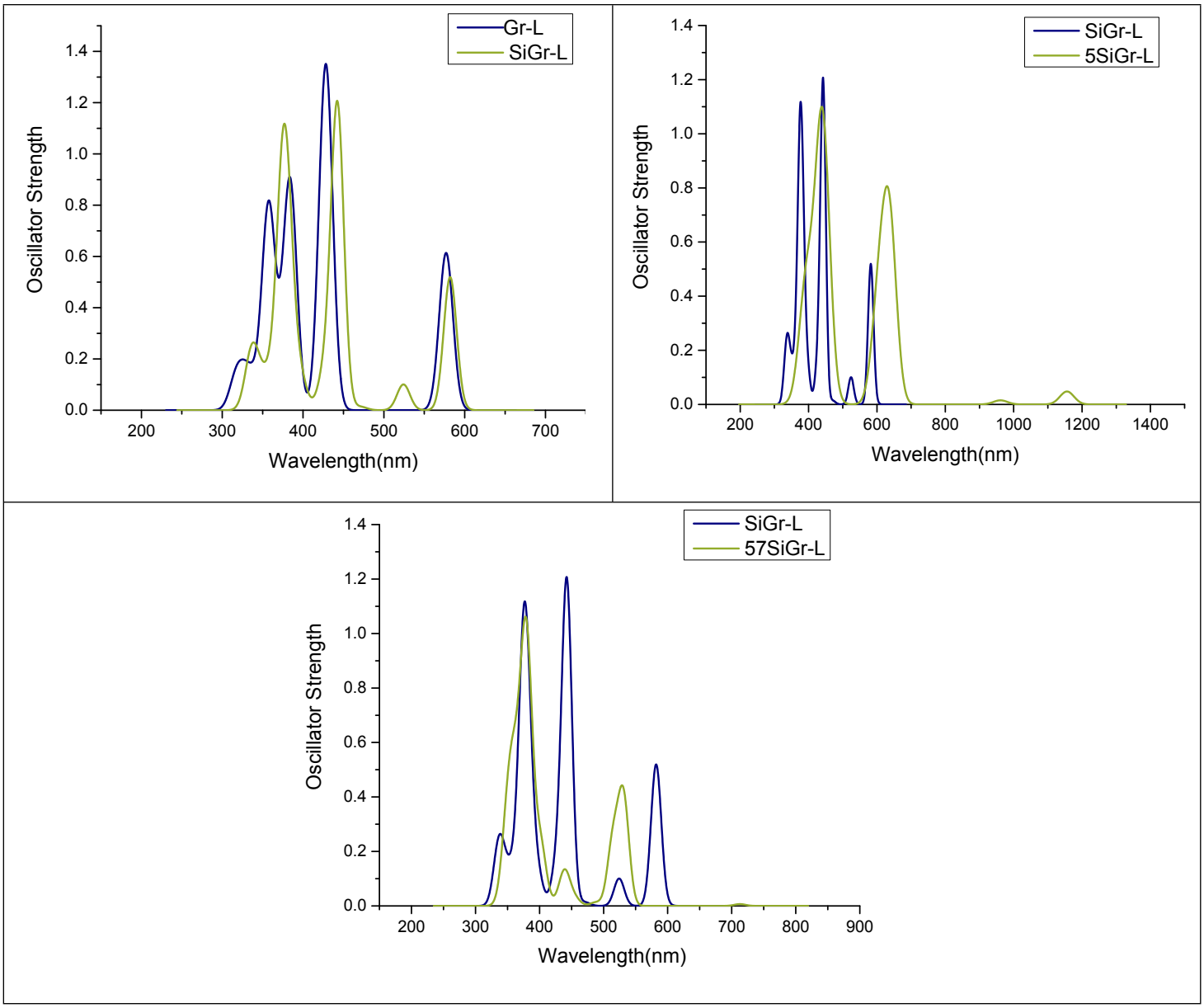
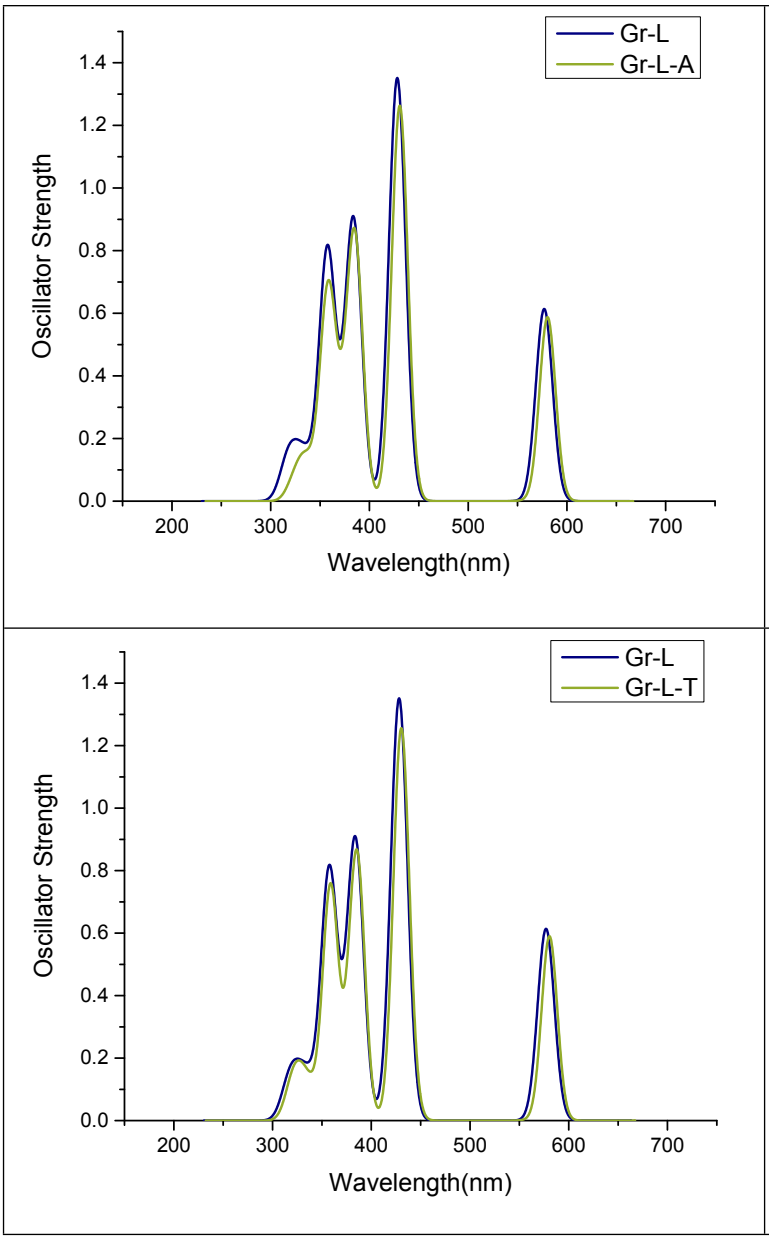
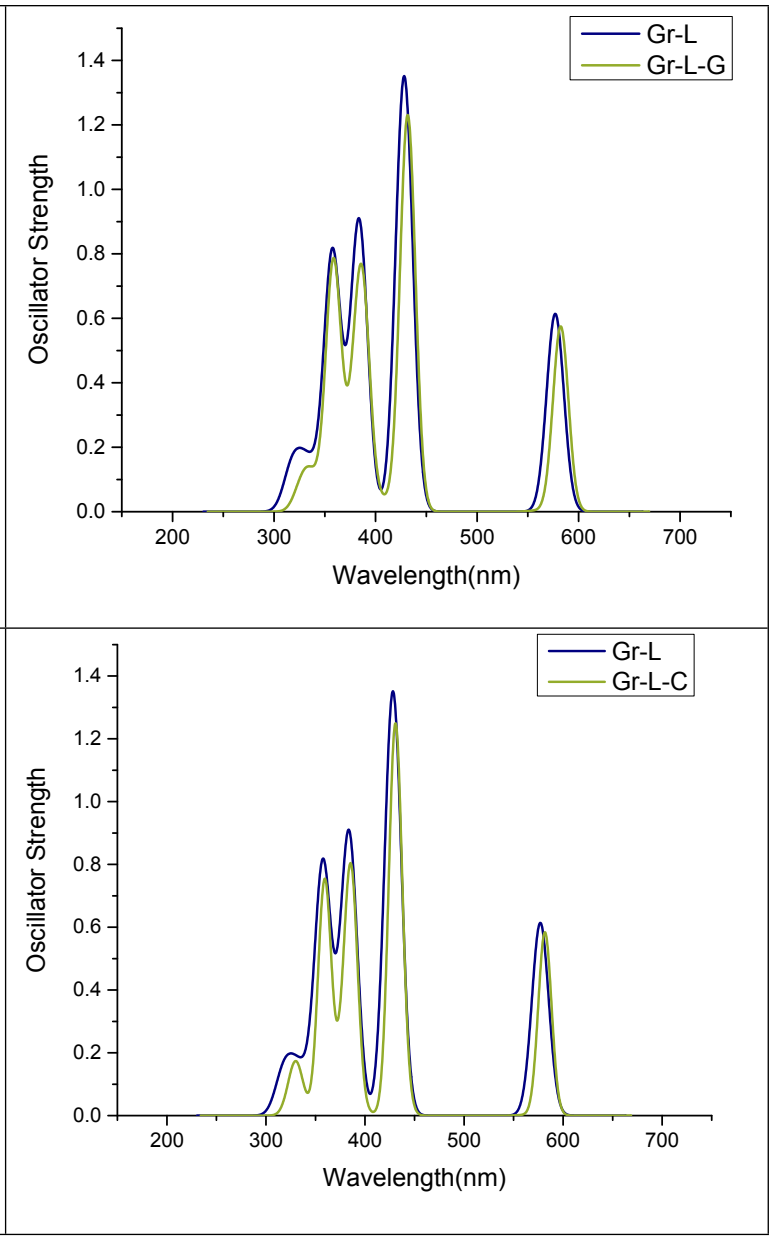


Fig. S6 The simulated absorption spectrum of Gr-L, SiGr-L, 5SiGr-L and 57SiGr-L at M06-2X/6-31G** level of theory.


Gr-L
Gr-L-A
Oscillator Strength
Wavelength(nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
200
300
400
500
600
700


Gr-L
Gr-L-G
Oscillator Strength
Wavelength(nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
200
300
400
500
600
700

Gr-L
Gr-L-T
Oscillator Strength
Wavelength(nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
200
300
400
500
600
700

Gr-L
Gr-L-C
Oscillator Strength
Wavelength(nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
200
300
400
500
600
700

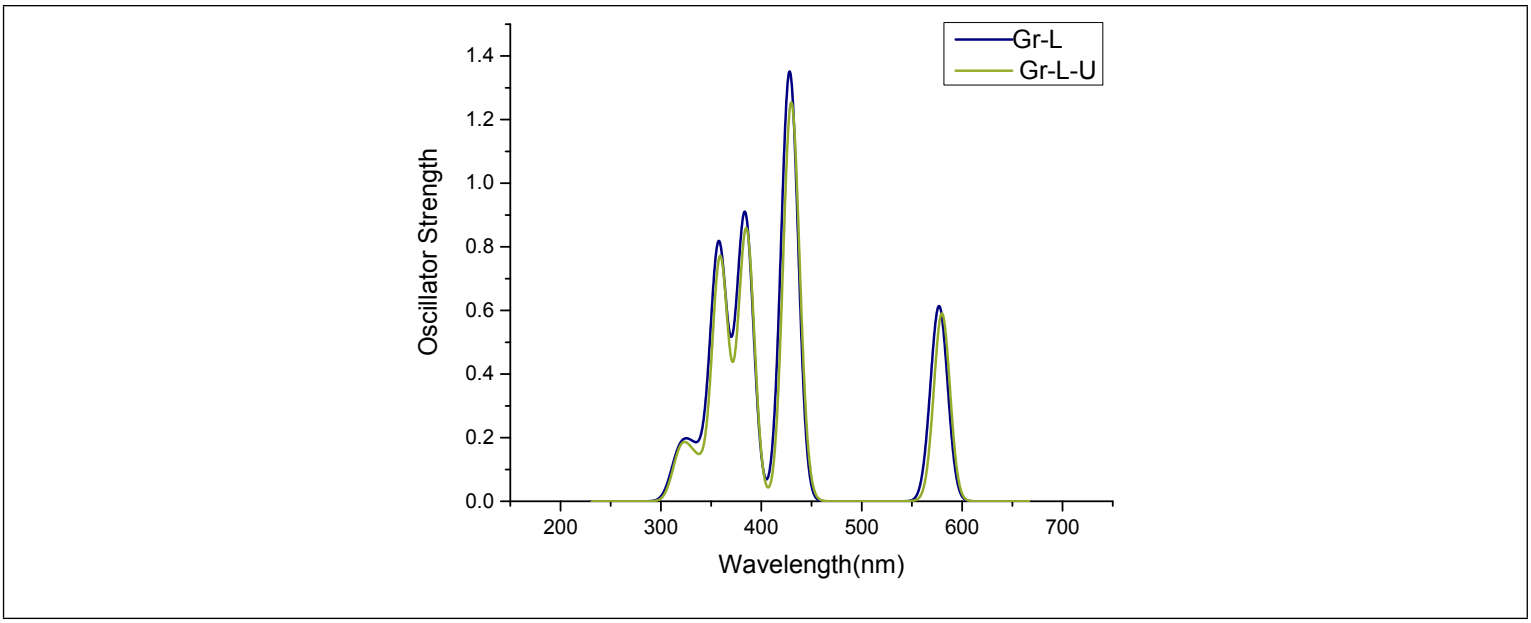
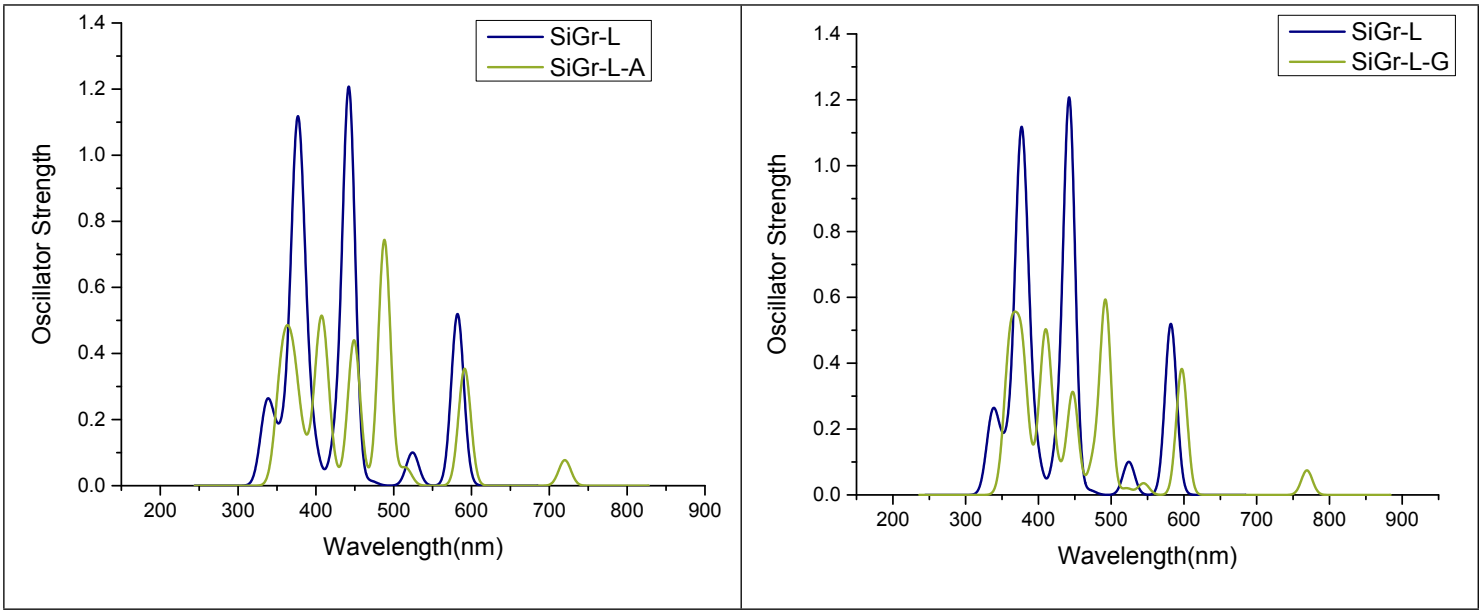
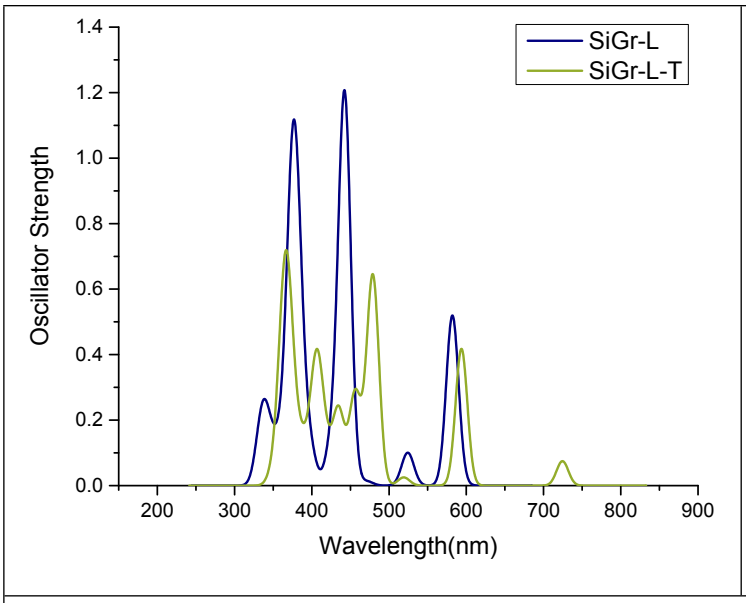
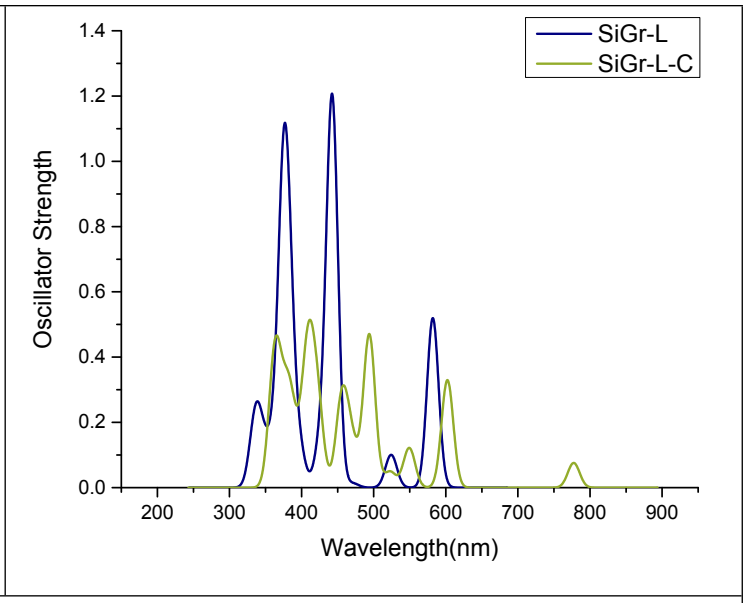
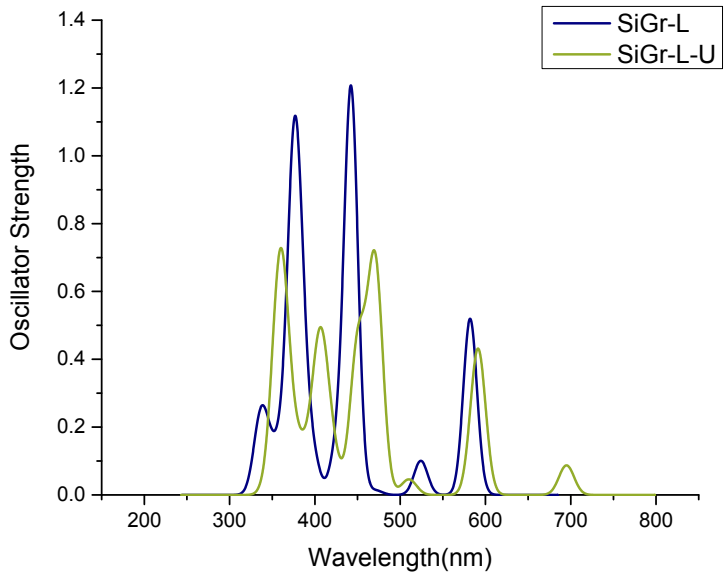


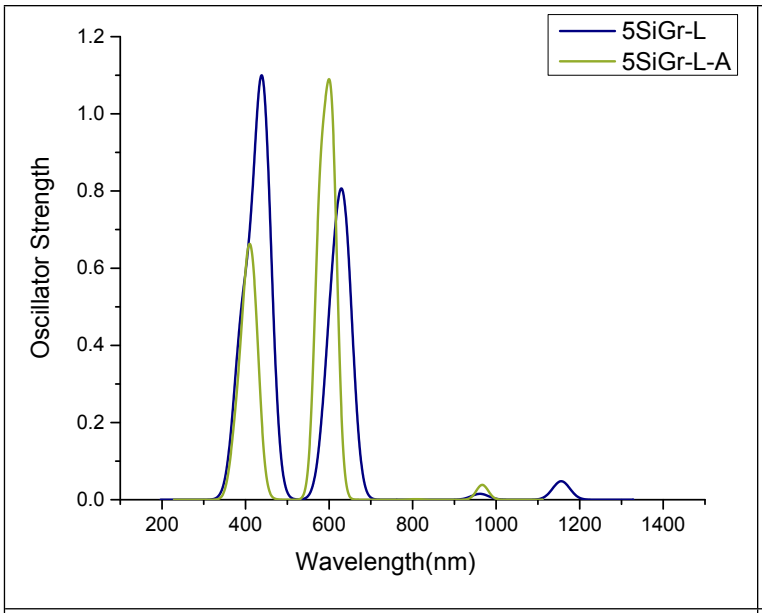
Fig. S7 The simulated absorption spectrum of the complexes of nucleobases with Gr-L at M06-2X/6-31G** level of theory.

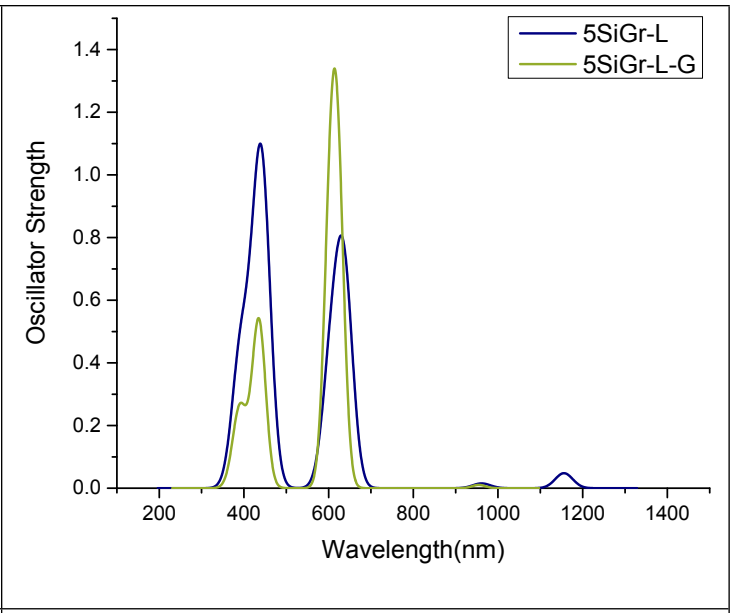


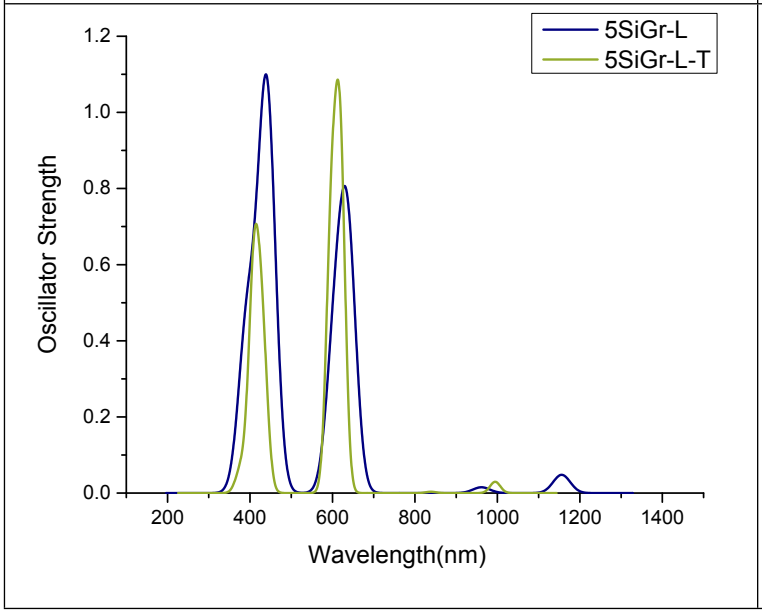

SiGr-L
SiGr-L-T
Oscillator Strength
Wavelength(nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
200
300
400
500
600
700
800
900

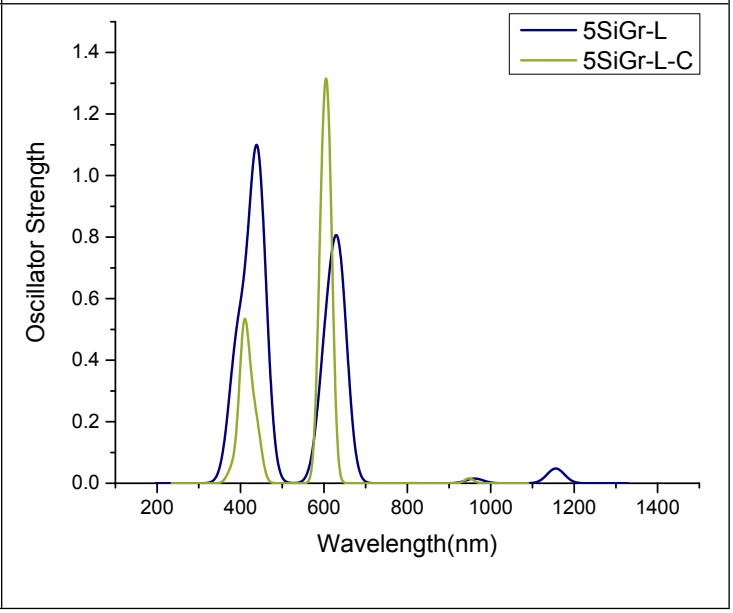

SiGr-L
SiGr-L-C
Oscillator Strength
Wavelength(nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
200
300
400
500
600
700
800
900


SiGr-L
SiGr-L-U
Oscillator Strength
Wavelength(nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
200
300
400
500
600
700
800


5SiGr-L
5SiGr-L-A
Oscillator Strength
Wavelength(nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
200
400
600
800
1000
1200
1400


5SiGr-L
5SiGr-L-G
Oscillator Strength
Wavelength(nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
200
400
600
800
1000
1200
1400


5SiGr-L
5SiGr-L-T
Oscillator Strength
Wavelength(nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
200
400
600
800
1000
1200
1400


5SiGr-L
5SiGr-L-C
Oscillator Strength
Wavelength(nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
200
400
600
800
1000
1200
1400

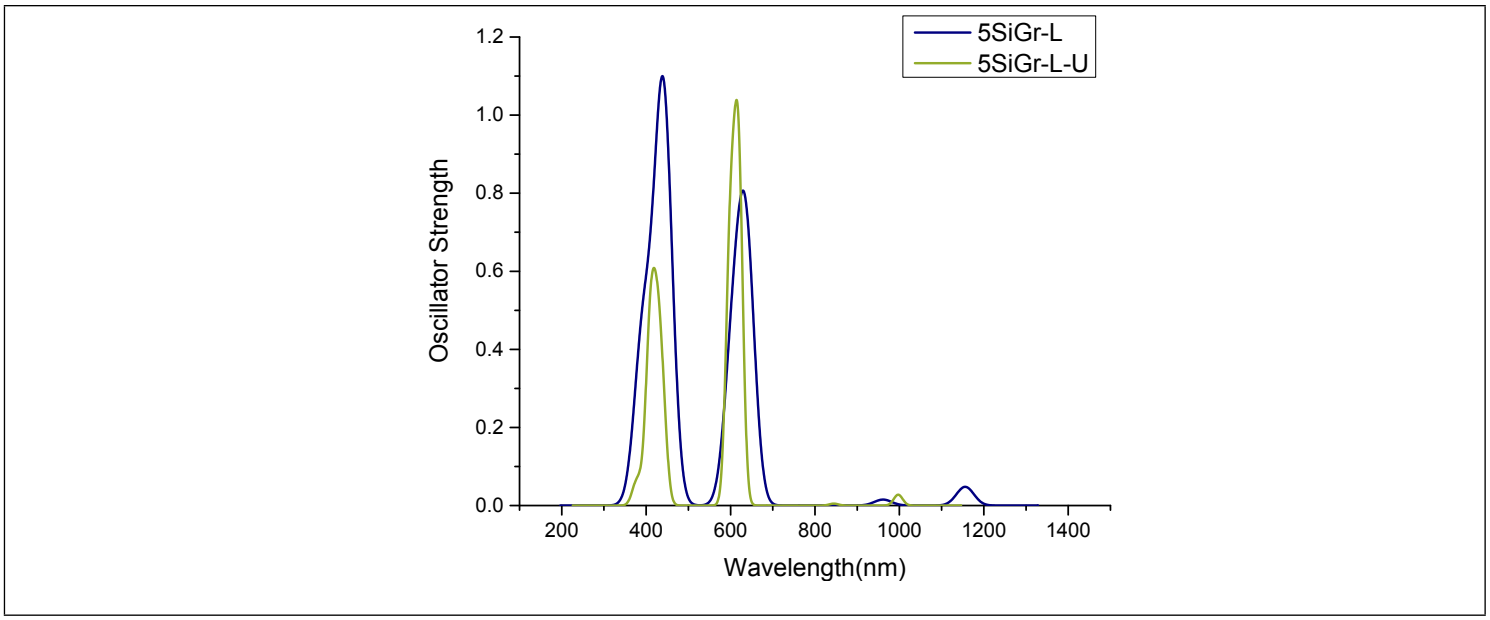
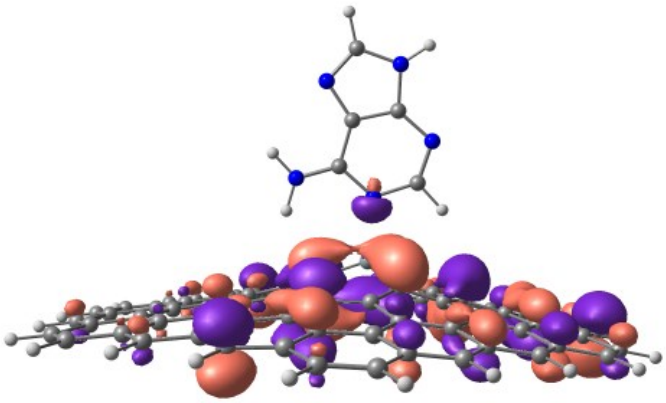
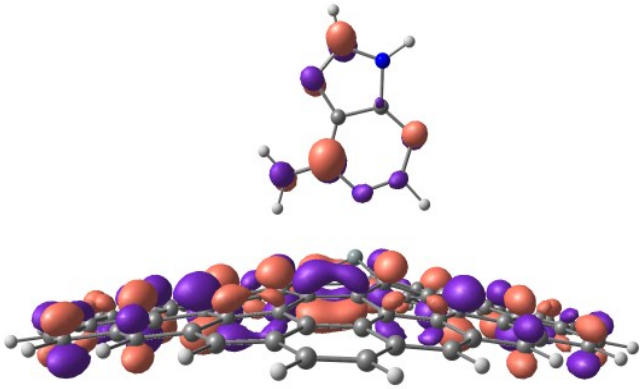
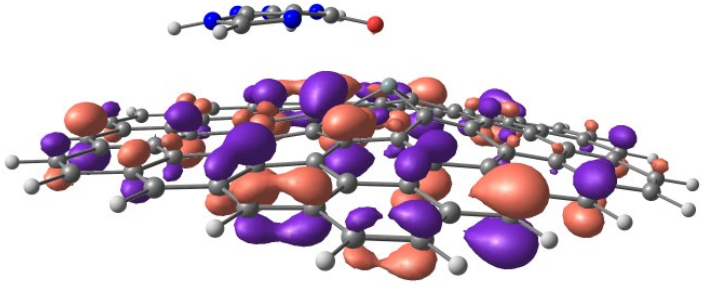
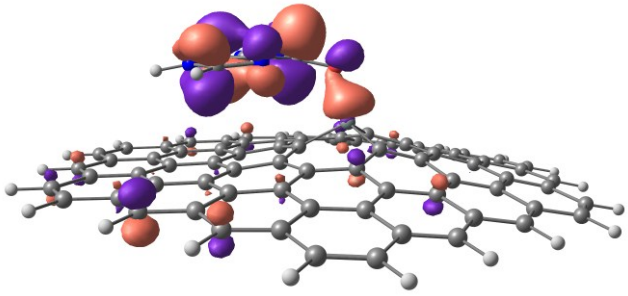
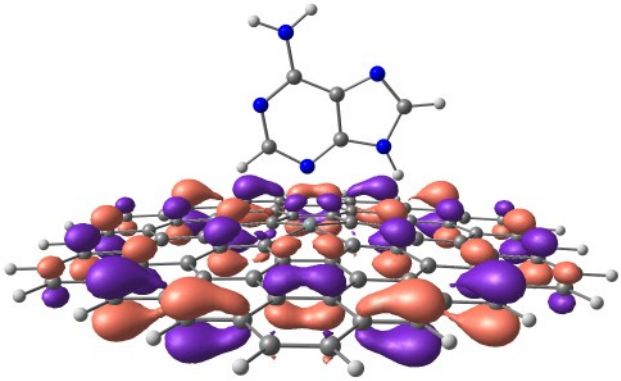
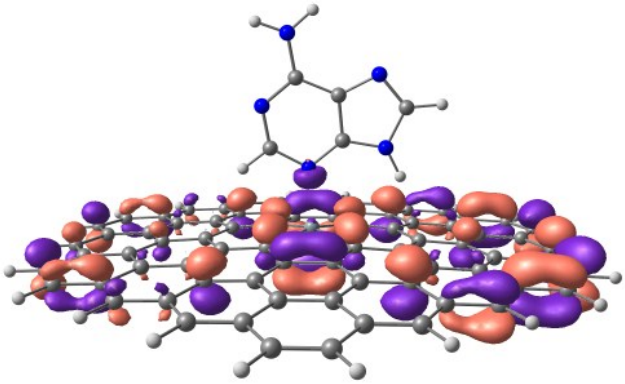
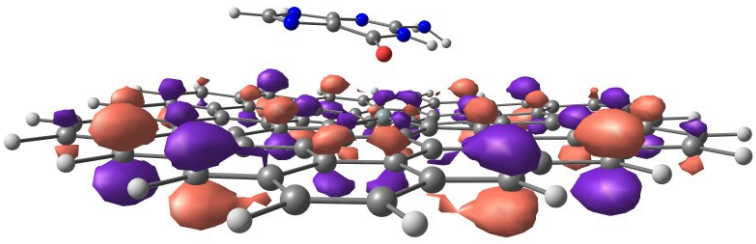
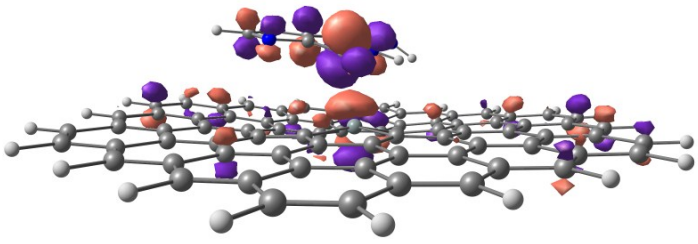
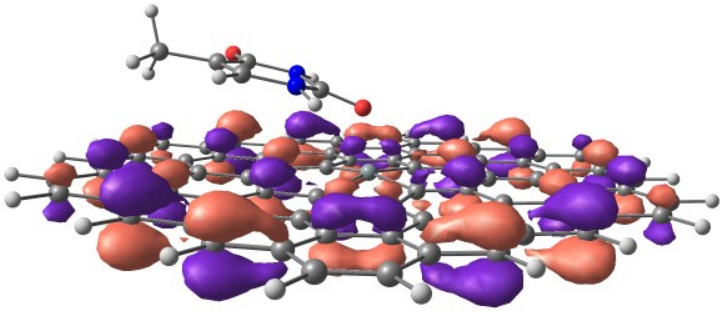
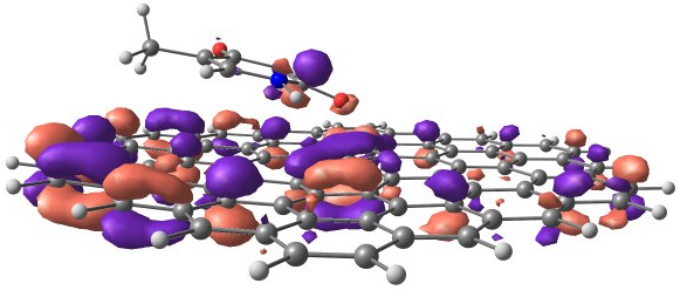


Fig. S8 The simulated absorption spectrum of the complexes of nucleobases with SiGr-L and 5SiGr-L at M06-2X/6-31G** level of theory.

 SiGr-L-A HOMO	 LUMO+7
 SiGr-L-G HOMO-2	 LUMO+2
 5SiGr-L-A HOMO	 LUMO+3
 5SiGr-L-G HOMO	 LUMO+3



5SiGr-L-T HOMO



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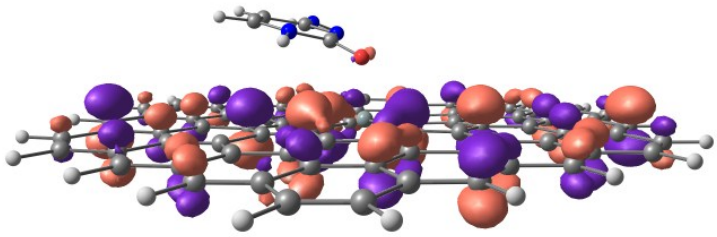
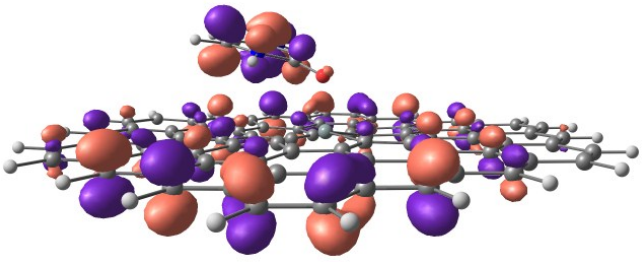


HOMO-1

5SiGr-L-C



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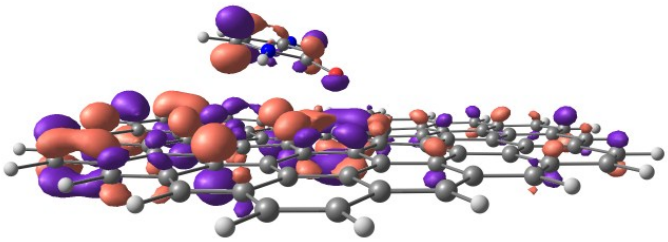
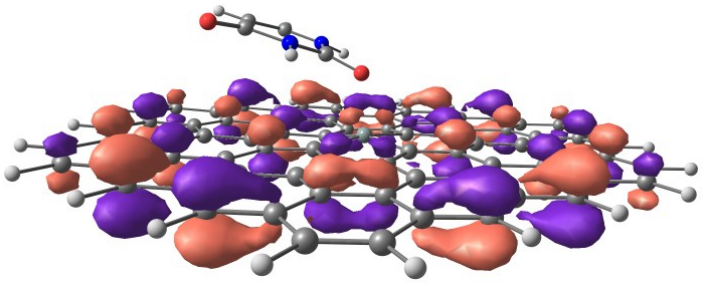
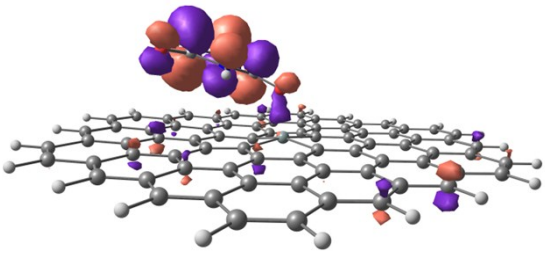


LUMO+4



HOMO

5SiGr-L-U



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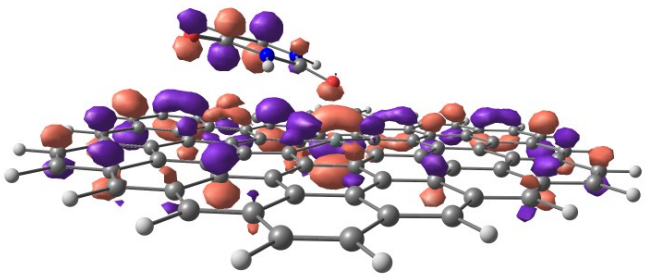

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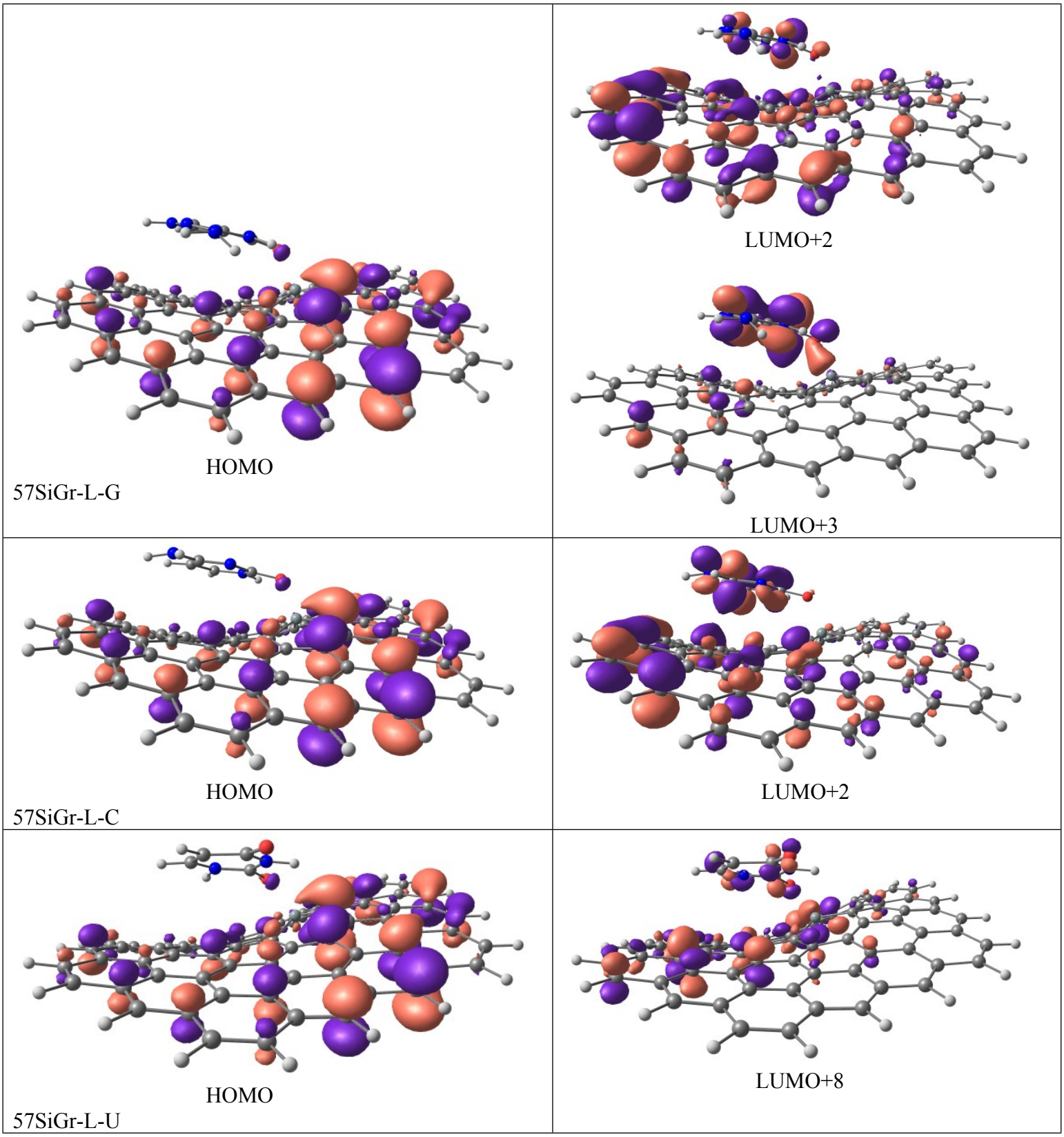

Fig. S9 The contour pictures of orbital involved in the transitions modified with NBs.