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

Electronic Supplementary Information

Molecular Charge Transfer by Adsorbing the TCNQ/TTF Molecules via π-π Interaction: A Simple and Effective Strategy to Modulate the Electronic and Magnetic Behaviors of Zigzag SiC Nanoribbons

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(I) Computational details of structure optimization

In this study, all the geometry structures are fully optimized. Specifically, considering the studied object is the one-dimensional nanoribbon, we employ the keyword "ISIF=2" to avoid the deformation of cell shape, and then we change the parameters of cell step by step to perform the optimization of geometry and make it satisfy the standard of full relaxation at last. Table S1 shows all the computational details of the structure optimization at the ferromagnetic (FM) state. For the nonmagnetic (NM) and antiferromagnetic (AFM) configurations, their details are only a slightly different from that of the corresponding FM state, that is, "ISPIN=1" should be used for NM state instead of "ISPIN=2", whereas the MAGMOM should be added to set the initial magnetic moment for the AFM state.

Table S1. Computational details of the structure optimization of the ferromagnetic (FM) configuration.

Keywords	Setting	Keywords	Setting	Keywords	Setting	Keywords	Setting
ISTART	0	GGA	PE	NELMIN	2	LWAVE	.FALSE.
ICHARG	2	ISPIN	2	EDIFF	1.00E-04	LCHARG	.FALSE.
IBRION	2	PREC	Medium	LVDW	.TRUE.	IALGO	48
ISIF	2	ENCUT	400	ISMEAR	0	LORBIT	11
NSW	100	NELM	100	SIGMA	0.02	LREAL	Auto

(II) Magnetic moments of the modified zSiCNR systems with the adsorbate TCNQ/TTF molecules

Table S2. The total magnetic moment M_{tot} (μB) for the ground state of the TCNQ-modified zSiCNR-complexes. The FM and AFM represent the ferromagnetic and antiferromagnetic spin couplings, respectively.

Systems	Ground state	M_{tot} (μB)
8-zSiCNR	FM/AFM	3.430/0.000
TCNQ-*a*(I)	FM	4.187
TCNQ-*a*(II)	FM	4.357
TCNQ-*a*(III)	AFM	0.000
TCNQ-*a*(IV)	FM	4.378
TCNQ-*b*(I)	FM	4.348
TCNQ-*b*(II)	FM	4.290
TCNQ-*b*(III)	FM	4.390
TCNQ-*b*(IV)	FM	4.480
TCNQ-*r*(I)	FM	4.417
TCNQ-*r*(II)	AFM	0.000
TCNQ-*r*(III)	FM	4.463
TCNQ-*r*(IV)	FM	4.460

Table S3. The total magnetic moment M_{tot} (μB) for the ground state of the TTF-modified zSiCNR-complexes. The FM and AFM represent the ferromagnetic and antiferromagnetic spin couplings, respectively.

Systems	Ground state	M_{tot} (μB)
TTF-*r*(I)	FM	3.415
TTF-*r*(II)	FM	3.420
TTF-*r*(III)	FM	3.416
TTF-*r*(IV)	FM	3.413
TTF-*b*(I)	AFM	0.000
TTF-*b*(II)	AFM	0.000
TTF-*b*(III)	FM	3.419

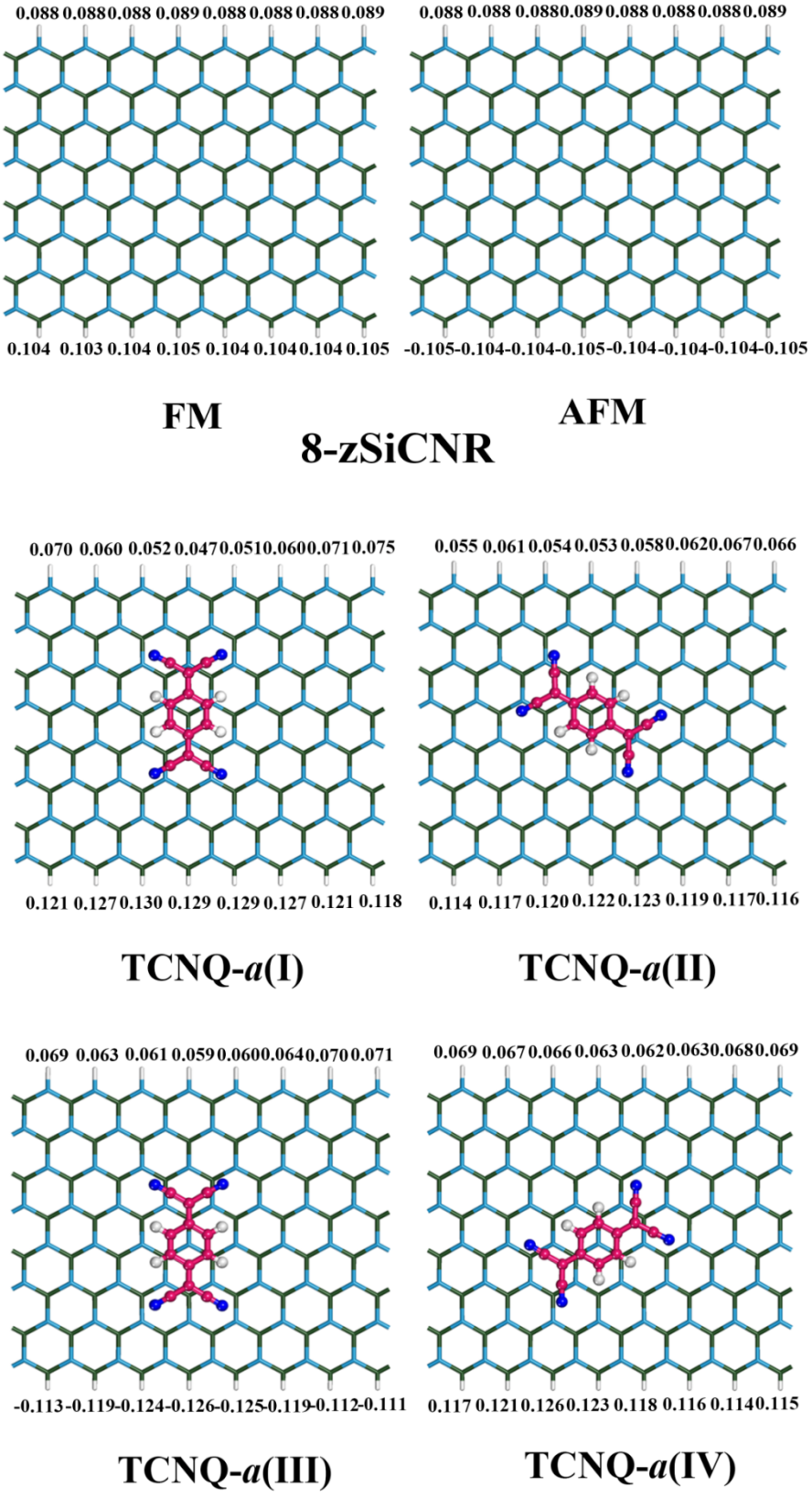
Table S4. The total magnetic moment M_{tot} (μB) for the ground state of the obtained zSiCNR-complexes by moving the adsorbed TCNQ molecule from the center towards the Si/C edges. The FM and AFM represent the ferromagnetic and antiferromagnetic spin couplings, respectively.

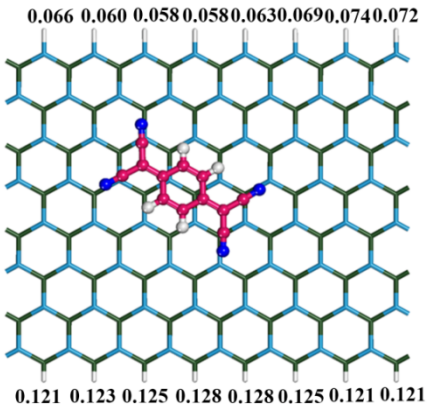
Systems	Ground state	M_{tot} (μB)
TCNQ-*a*(I)	FM	4.187
TCNQ-*a*(I)-eSi-s1	AFM	2.000
TCNQ-*a*(I)-eSi-s2	AFM	2.000
TCNQ-*a*(I)-eC-s1	AFM	0.000
TCNQ-*a*(I)-eC-s2	AFM	0.000

Table S5. The total magnetic moment M_{tot} (μB) for the ground state of the obtained zSiCNR-complexes by moving the adsorbed TTF molecule from the center towards the Si/C edges. The FM and AFM represent the ferromagnetic and antiferromagnetic spin couplings, respectively.

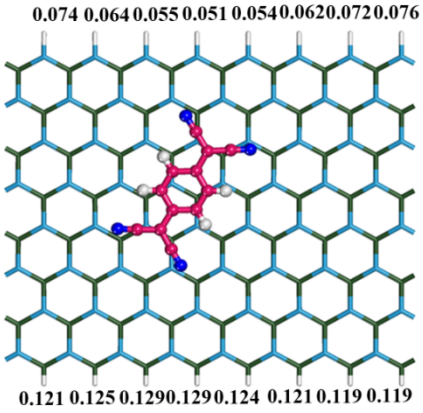
Systems	Ground state	M_{tot} (μB)
TTF-*r*(I)	FM	3.415
TTF-*r*(I)-eSi-s1	FM	3.416
TTF-*r*(I)-eSi-s2	FM	3.432
TTF-*r*(I)-eC-s1	FM	3.434
TTF-*r*(I)-eC-s2	FM	3.482

Figure S1. The magnetic moment M (μB) on the edge C/Si atoms for the zSiCNR-complexes with adsorbing the TCNQ molecule at the different sites in the center.

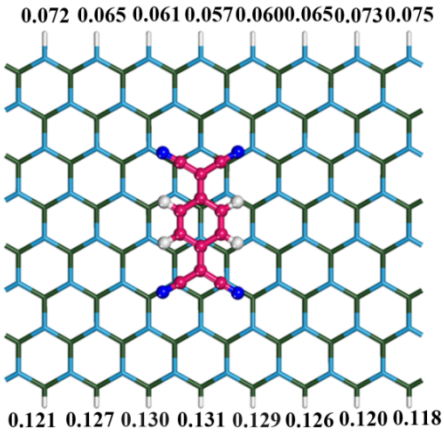




TCNQ-*b*(I)



TCNQ-*b*(II)



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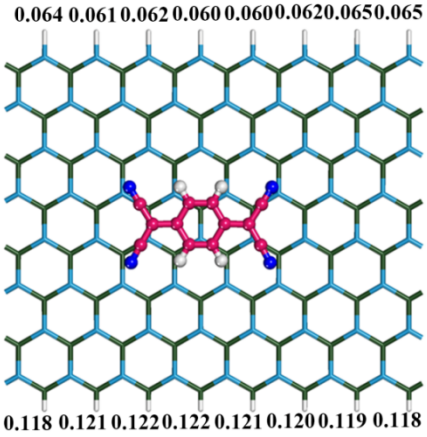
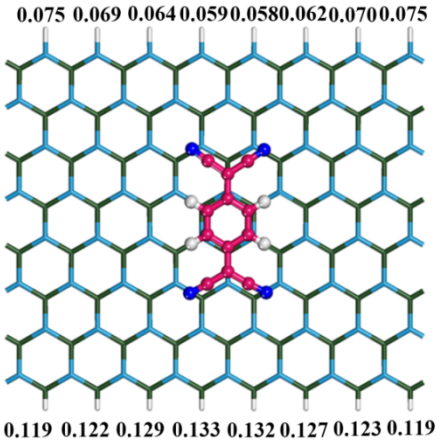
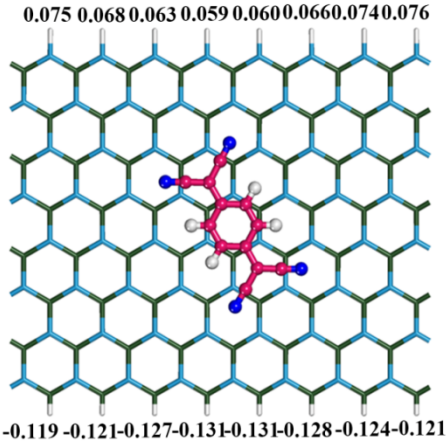


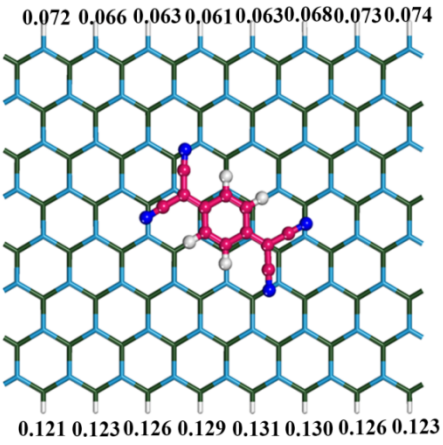
TCNQ-*b*(IV)



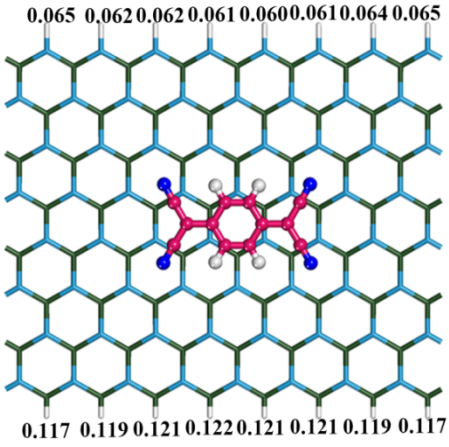
TCNQ-*r*(I)



TCNQ-*r*(II)

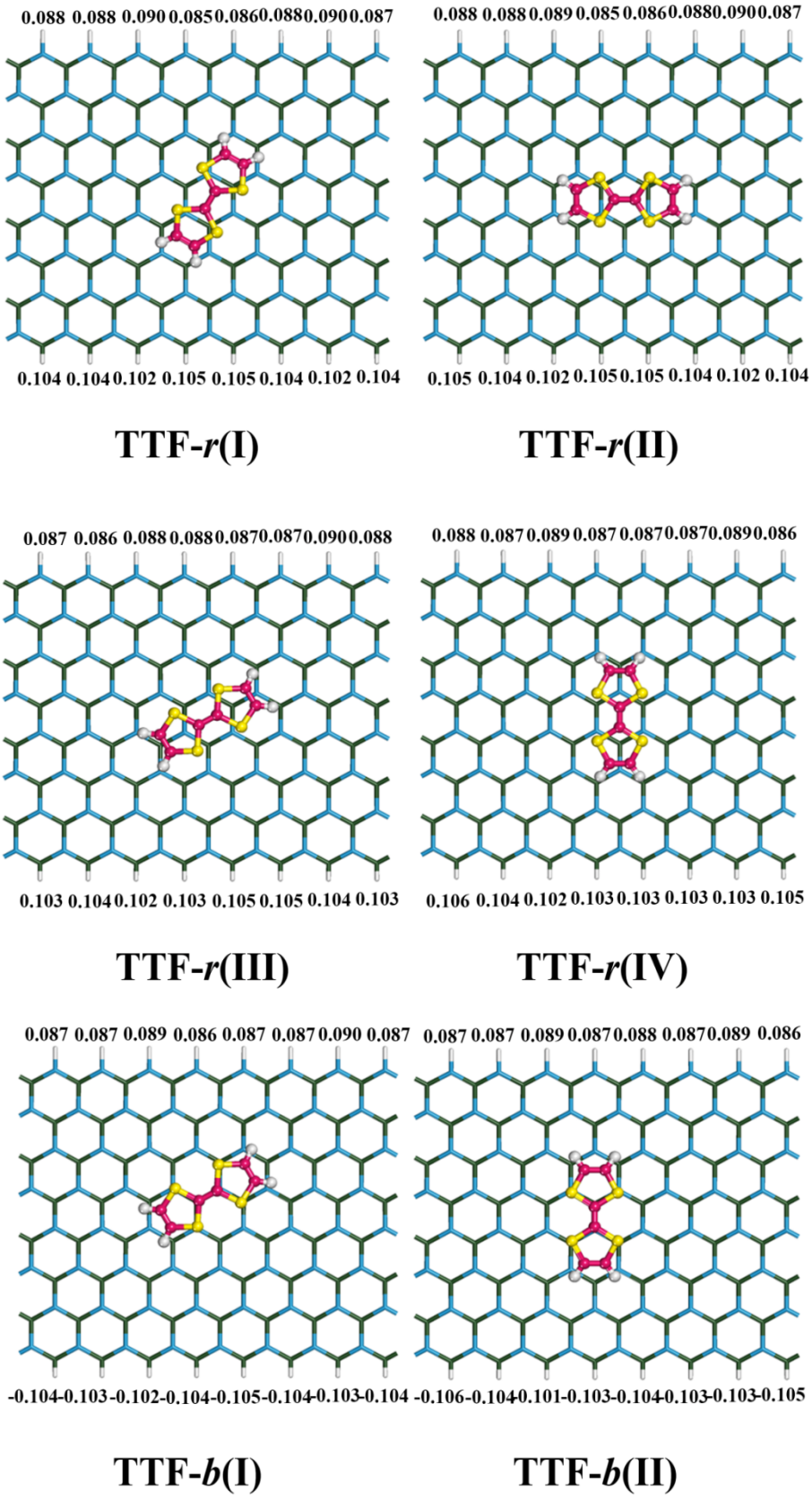


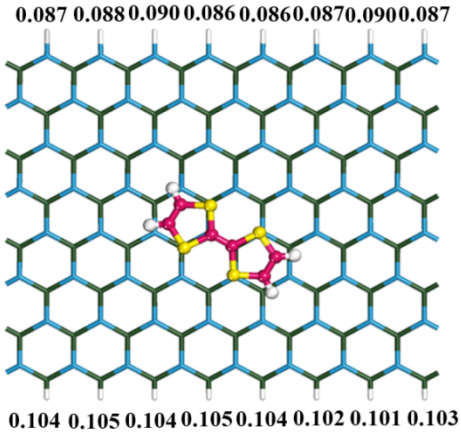
TCNQ-*r*(III)



TCNQ-*r*(IV)

Figure S2. The magnetic moment M (μB) on the edge C/Si atoms for the zSiCNR-complexes with adsorbing the TTF molecule at the different sites in the center.




0.087 0.088 0.090 0.086 0.086 0.087 0.090 0.087
0.104 0.105 0.104 0.105 0.104 0.102 0.101 0.103

TTF-*b*(III)

Figure S3. The magnetic moment M (μB) on the edge C/Si atoms for the obtained zSiCNR-complexes by moving the adsorbate TCNQ from the center towards the Si/C edges.

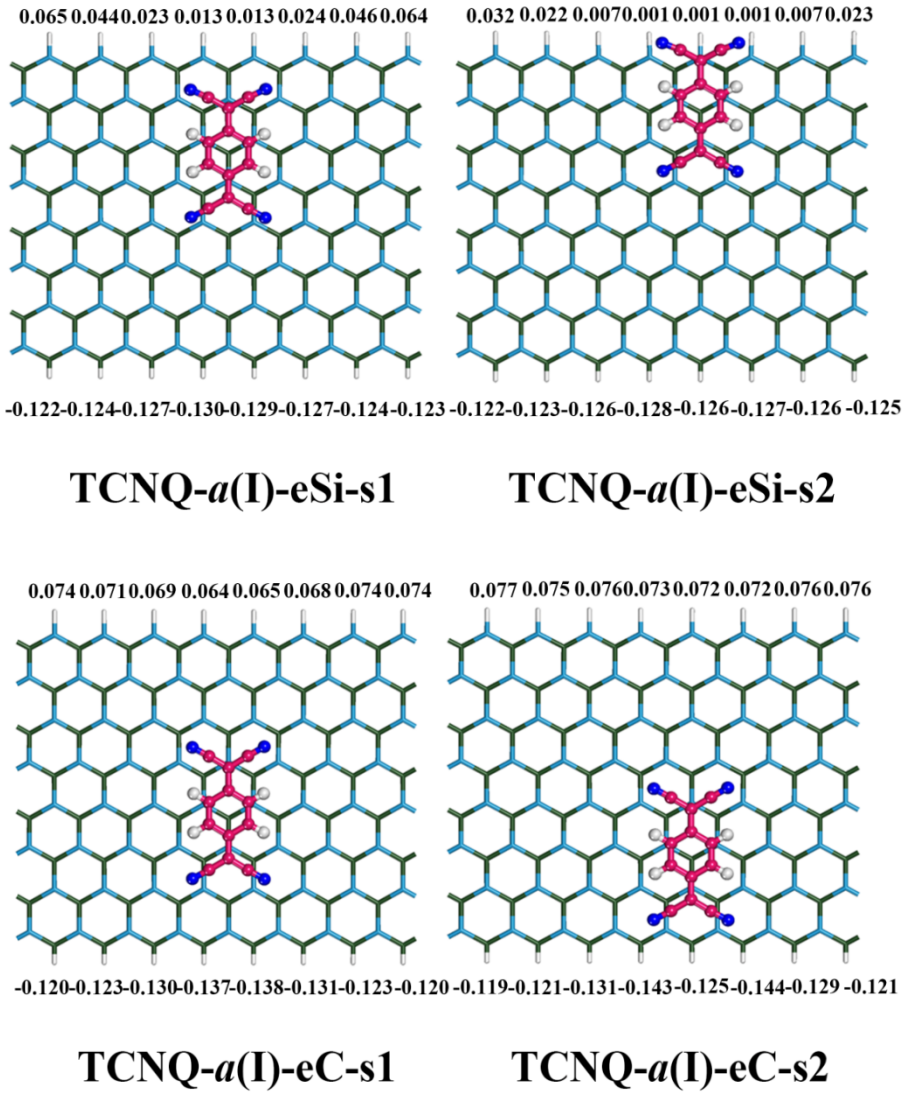


Figure S4. The magnetic moment M (μB) on the edge C/Si atoms for the obtained zSiCNR-complexes by moving the adsorbate TTF from the center towards the Si/C edges.