Supporting Information

Doping Effect on Edge Terminated Ferromagnetic Graphene Nanoribbons

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Table of Contents

Figure S1. Spin distribution patterns of (un)doped of TZT calculated with PBE0 functional.

Table S1. Electronic energy difference and magnetic moment of **TZT** calculated with PBE0 functional.

Scheme S1. Schematic diagram of Major coupling pathway, specific doping position and atoms in edge and radical for TZT, OZO and TZO.

Table S2. Electronic energy difference and magnetic moment of each doped TZT, OZO, and TZO

Figure S2. Comparison of magnetic ground state of BN-doped TZT depending on doping position.

Table S3. Electronic energy difference and magnetic moment of BN-doped TZT for different doping position.

Table S4. Atomic mangetization, bond length, dihedral angle, coupler length of TZO system.

Figure S3. Density of states diagram for undoped and doped TZT system.

Figure S4. Spin distribution patterns of doped and undoped TZT system at B and N doped geometry.

Figure S5. Density of states diagram for undoped and doped OZO system.

Figure S6. Density of states diagram for undoped and doped TZO system.

PBE0

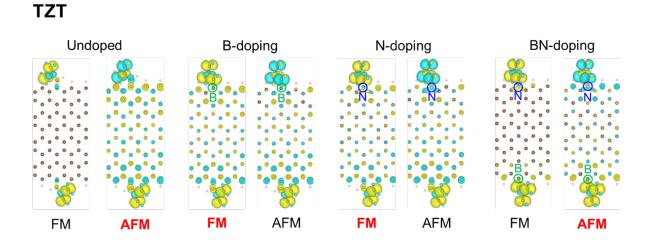
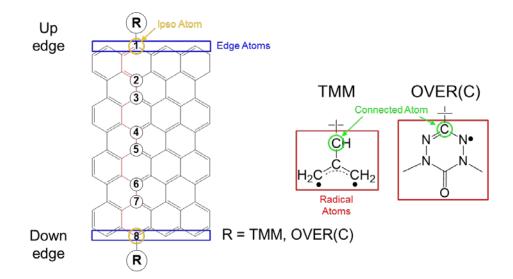


Figure S1. Spin distribution patterns of doped and undoped **TZT** system. Yellow and cyan colors represent up and down spin respectively. The B or N doping positions are marked in green or blue circle, respectively. More stable configurations were marked in red.

Table S1. Energy Differences between FM and AFM Configurations (ΔE_{FM-AFM} , in meV), Net Magnetic Moment per Unit Cell (μ_s , in μ_B) of **TZT** system. Calculated with PBE0 Functional.

	undoped		B-de	B-doped N-doped		oped	BN-doped	
	FM	AFM	FM	AFM	FM	AFM	FM	AFM
ΔE_{FM-AFM}	26.740		-19.	.320	-15.	.150	13.	580
$\mu_{s}\left(\mu_{B} ight)$	1.999	0.000	3.000	-1.000	3.000	-1.000	4.001	0.000



Scheme S1. Schematic diagram of major spin coupling pathway (red line), B- or N-doped position (18) for TZT, OZO, and TZO, and specific atom: ipso atom of edge and connected atom of radical.

	TZT									
-	B-1 ^b	B-2	B-3	B-4	N-1	N-2	N-3	N-4		
ΔE_{FM-AFM}	-0.290	-0.040	-0.070	-0.070	-0.002	-0.170	-0.080	-0.060		
$\mu_{s}(FM)$	2.945	1.958	1.970	1.964	2.976	1.922	1.956	1.949		
μ_s (AFM)	-0.982	0.006	-0.035	0.008	-1.011	0.031	-0.016	0.012		
_	OZO									
	B-1	B-2	B-3	B-4	N-1	N-2	N-3	N-4		
ΔE_{FM-AFM}	-0.840	-1.120	-1.580	-3.890	-1.730	-1.590	-0.200	-1.420		
$\mu_s(FM)$	2.837	3.341	3.489	3.663	2.768	3.064	3.141	3.369		
μ_s (AFM)	0.897	0.486	0.410	0.091	0.991	0.598	0.490	0.0190		
_				TZO	О-В					
	B-1	B-2	B-3	B-4	B-5	B-6	B-7	B-8		
ΔE _{FM-AFM}	1.140	0.340	0.840	0.400	0.700	0.320	0.340	0.250		
$\mu_{s}(FM)$	3.786	2.812	2.898	2.728	2.812	2.509	2.404	1.945		
μ_s (AFM)	-0.042	0.887	0.927	0.784	0.846	0.578	0.458	-0.023		
	TZO-N									
	N-1	N-2	N-3	N-4	N-5	N-6	N-7	N-8		
ΔE _{FM-AFM}	0.550	0.310	0.570	0.330	0.410	0.050	0.220	1.050		
$\mu_{s}(FM)$	3.831	2.757	2.812	2.651	2.635	2.291	2.190	1.855		
μ_{s} (AFM)	-0.128	0.834	0.833	0.706	0.667	0.341	0.234	-0.108		

(ΔE_{FM-AFM} , in meV), Net Magnetic Moment per Unit Cell (μ_s , in μ_B) of B- and N-doped system along with major spin coupling pathway for **TZT**, **OZO**, and **TZO**. Calculated with PBE Functional.^{*a*}

Table S2. Calculated Electronic Energy Difference between FM and AFM Magnetic Configurations

^{*a*} Only 1-4 doping position was calculated for **TZT** and **OZO** system due to symmetry.

^b B (or N)-n indicates B (or N) doping at n position depicted in Scheme S1.

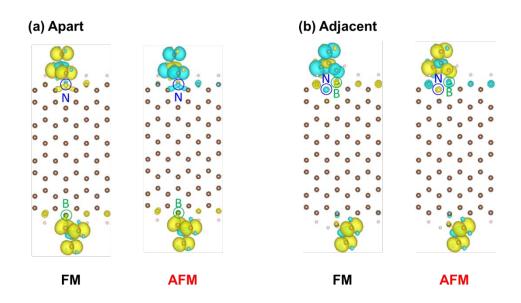


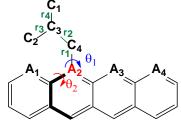
Figure S2. Comparison of magnetic ground state of BN-doped **TZT** system depending on the doping position of B and N atom. (a) B and N apart (b) B and N adjacent. Ground spin configuration were marked in red.

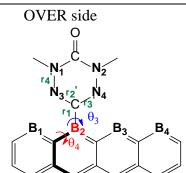
Table S3. Calculated Electronic Energy Difference between FM and AFM Magnetic Configurations (ΔE_{FM-AFM} in meV), Net Magnetic Moment per Unit Cell (μ_s in μ_B) of B- and N-Doped System for Doping Position. Calculated with PBE Functional

	undo	oped	BN aj	part	BN adj	BN adjacent	
	FM	AFM	FM	AFM	FM	AFM	
ΔE_{FM-AFM}	0.330		0.28	0.280		0.800	
$\mu_{s}\left(\mu_{B} ight)$	1.964	0.001	3.951	0.040	2.082	0.116	

Table S4. Atomic Magnetizations ($\mu(X_i)$ where X = C, N, A, and B in 0.0001 μ_B) on radical (C_n or N_n) and Edge Atoms (A_n or B_n) Compared to Undoped System by Doping (Atom Magnetizations of Undoped System were Written in Brackets: [C_n , N_n]) for TZO, Selected Bond Lengths (r1- r4 and r1'- r4' in Å), Dihedral Angle between TMM Radical and Ipso Atom against ZGNR Coupler ($\theta_1 - \theta_4$ in °), and Coupler Length (d, in Å) between radicals. The Values for B-TMM/N-OVER and N-TMM/B-OVER Systems Represent Those for B/N and N/B Edge, Respectively.

				TZO					
	undoped	B-TMM	B-OVER	N-TMM	N-OVER	B-TMM /N-OVER	N-TMM /B-OVER		
$C_1(N_1)$	0 [175,160]	4	-16	36	-28	37 (-28)	45 (-18)		
$C_2(N_2)$	0 [196,160]	31	-13	35	-29	22 (-29)	35 (-11)		
C ₃ (N ₃)	0 [48,103]	6	-1	7	-4	4 (-4)	9 (-2)		
$C_4(N_4)$	0 [9,103]	169	0	194	-4	162 (-5)	204 (0)		
$A_1(B_1)$	0 [6,77]	7	-76	5	-75	13 (-73)	7 (-75)		
$A_2(B_2)$	0 [8,95]	-3	-94	7	-93	12 (-93)	2 (-94)		
A ₃ (B ₃)	0 [7,77]	9	-75	5	-75	17 (-73)	1 (-74)		
$A_4(B_4)$	0 [1,81]	6	-79	-4	-78	13 (-75)	4 (-77)		
r1(r1')	1.36 (1.50)	1.53 (1.50)	1.36 (1.63)	1.39 (1.50)	1.36 (1.45)	1.53 (1.45)	1.40 (1.62)		
r2(r2')	1.49 (1.35)	1.44 (1.35)	1.49 (1.35)	1.43 (1.35)	1.49 (1.34)	1.45 (1.34)	1.43 (1.35)		
r3(r3')	1.40 (1.35)	1.41 (1.35)	1.40 (1.35)	1.41 (1.35)	1.40 (1.34)	1.41 (1.34)	1.41 (1.35)		
r4(r4')	1.39 (1.35)	1.41 (1.35)	1.39 (1.36)	1.40 (1.35)	1.39 (1.36)	1.41 (1.36)	1.41 (1.36)		
θ_1	52.43	52.81	52.40	63.07	52.16	52.30	64.42		
θ_2	11.05	7.86	10.89	8.91	10.98	9.10	7.62		
θ_3				~ 0					
θ_4				~ 0					
d	28.60	28.87	28.87	28.55	28.60	28.81	28.78		
		TMM si	de		OVER side				
						0			
	C₁				N C N				





TZT (a) undoped (b) B-doped FΜ AFM AFM FΜ 10 Spin up 10 Spin up B-doped Spin up B-doped Spin up Up Up Edge Edge Spin down PDOS PDOS Spin down Spin dowr E_F(0) -1.5 E_F(0) -1.5 E_F(0) -1.5 E_F(0) -1.5 +1 -1 +1 +1 -1 -1 -1 +1 10 10 Spin up Spin up Spin up Spin up Down Down Edge Edge Spin dowr Spin dowr Spin dowr -10 -10 -1.5 -1 E_F(0) +1 -1.5 -1 E_F(0) +1 - Total DOS -1.5 -1 E_F(0) +1 -1.5 -1 E_F(0) +1 - Radical Atoms - Edge Atoms (c) N-doped **BN-doped** (d) - Connected Atom - Ipso Atom 10 Spin up 10 Spin up N-doped N-doped N-doped Spin up Spin up N-doped Up Up Edge Edge Spin down Spin dowr PDOS Spin dowr Spin down PDOS 10 $E_F(0)$ -1.5 -1 E_F(0) -1.5 $E_F(0)$ -1.5 -1 E_F(0) -1.5 -1 +1 +1 -1 +1 +1 10 10 B-doped Spin up Spin up 🕈 Spin up Spin up B-doped Down Down Edge Edge Spin down Spin down Spin down Spin down -10 -10 -1.5 -1.5 -1 $E_F(0)$ +1 -1.5 -1 $E_F(0)$ +1 -1 $E_F(0)$ +1 -1.5 -1 E_F(0) +1

Figure S3. Density of States diagram for (a) undoped, (b) B-doped, (c) N-doped and (d) BN-doped **TZT** system. Each "Up edge" and "Down edge" includes both radical and edge atoms. Unfilled black line represents total DOS. Filled red, blue, green, and yellow represents DOS of total radical atoms, edge atoms, connected atom of radical, and ipso atom, respectively. (Scheme S1)

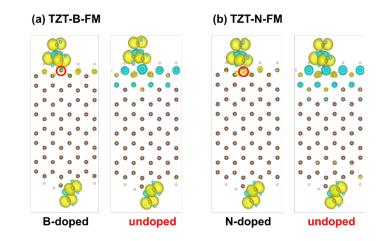


Figure S4. Spin distribution patterns of doped and undoped TZT system at B and N doped geometry obtained by PBE-vdW-DF calculations.

OZO

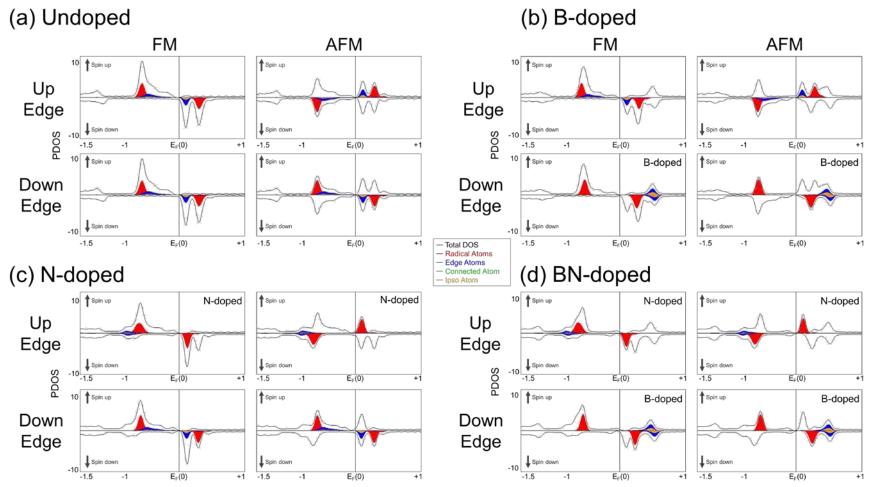


Figure S5. Density of States diagram for (a) undoped, (b) B-doped, (c) N-doped and (d) BN-doped **OZO** system. Each "Up edge" and "Down edge" includes both radical and edge atoms. Unfilled black line represents total DOS. Filled red, blue, green, and yellow represents DOS of total radical atoms, edge atoms, connected atom of radical, and ipso atom, respectively. (**Scheme S1**)

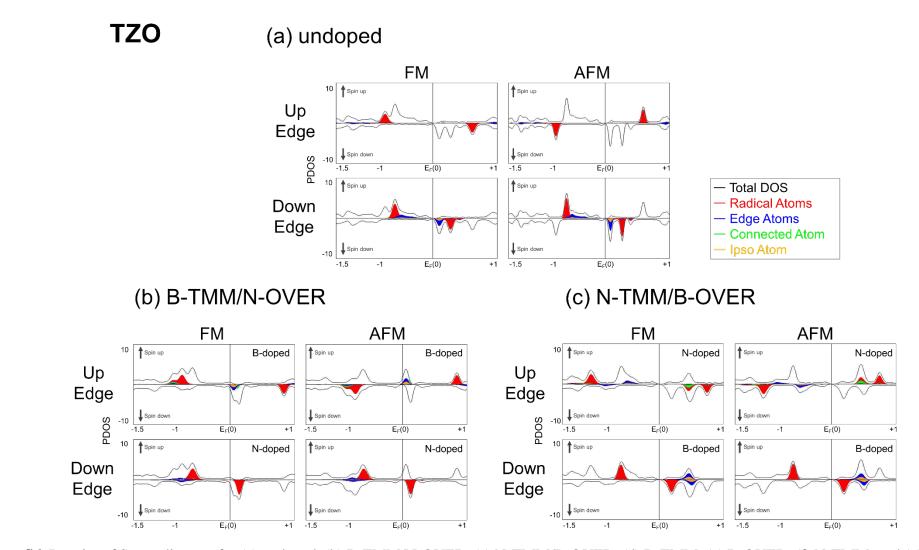


Figure S6. Density of States diagram for (a) undoped, (b) B-TMM/N-OVER, (c) N-TMM/B-OVER, (d) B-TMM, (e) B-OVER, (f) N-TMM, and (g) N-OVER **TZO** system. Each "Up edge" and "Down edge" includes both radical and edge atoms. Unfilled black line represents total DOS. Filled red, blue, green, and yellow represents DOS of total radical atoms, edge atoms, connected atom of radical, and ipso atom, respectively. (Scheme S1)

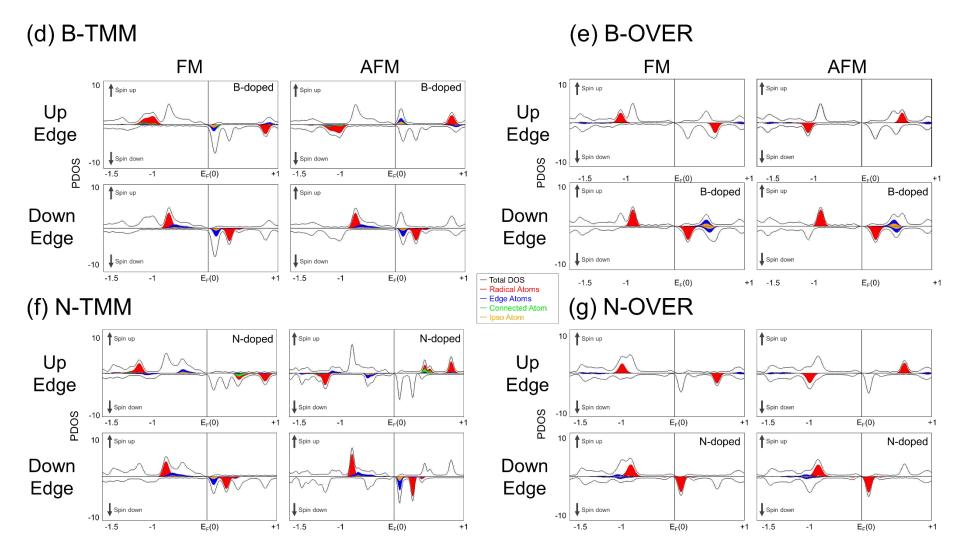


Figure S6. (Continued)