Supporting Information

Doping Effect on Edge Terminated Ferromagnetic Graphene Nanoribbons

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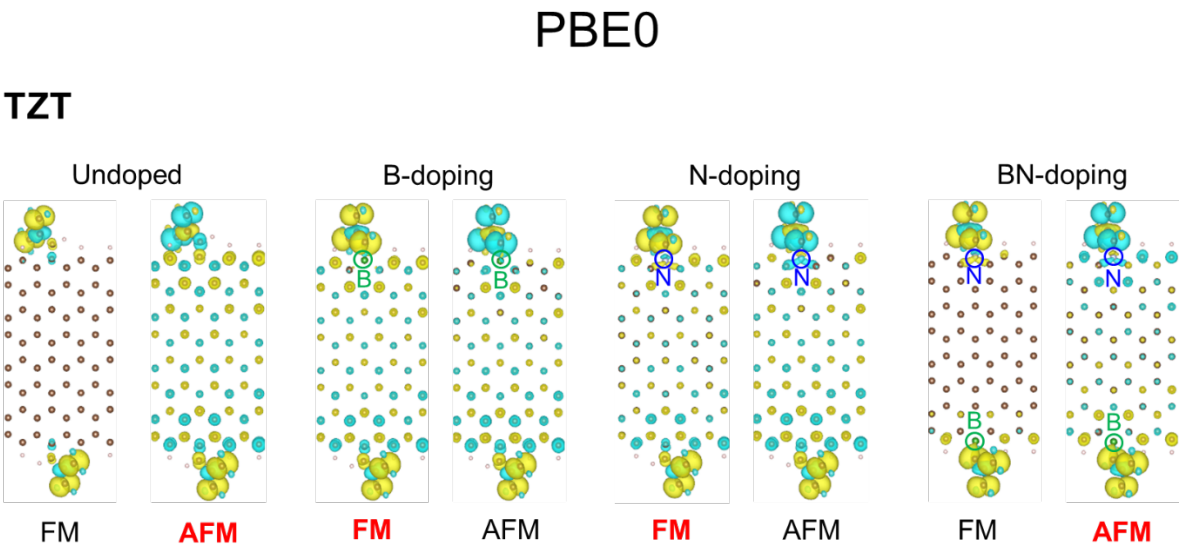
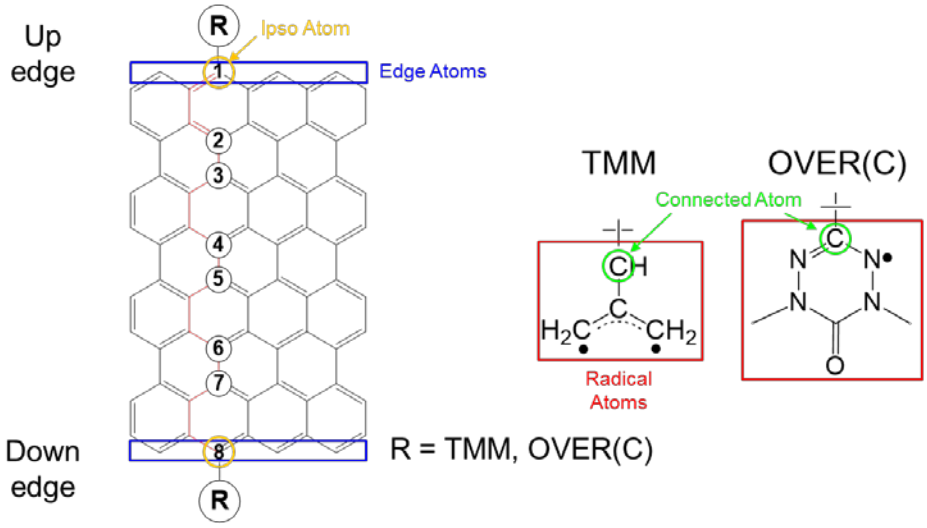


Figure S1. Spin distribution patterns of doped and undoped **TZT** system. Yellow and cyan colors represent up and down spin respectively. The B or N doping positions are marked in green or blue circle, respectively. More stable configurations were marked in red.

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

	undoped		B-doped		N-doped		BN-doped	
	FM	AFM	FM	AFM	FM	AFM	FM	AFM
$\Delta E_{FM\text{-}AFM}$	26.740		-19.320		-15.150		13.580	
μ_s (μ_B)	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 (1-8) for **TZT**, **OZO**, and **TZO**, and specific atom: ipso atom of edge and connected atom of radical.

Table S2. Calculated Electronic Energy Difference between FM and AFM Magnetic Configurations ($\Delta E_{FM\text{-}AFM}$, 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]

	TZT							
	B-1[b]	**B-2**	**B-3**	**B-4**	**N-1**	**N-2**	**N-3**	**N-4**
$\Delta E_{FM\text{-}AFM}$	-0.290	-0.040	-0.070	-0.070	-0.002	-0.170	-0.080	-0.060
μ_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**
$\Delta E_{FM\text{-}AFM}$	-0.840	-1.120	-1.580	-3.890	-1.730	-1.590	-0.200	-1.420
μ_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-B							
	B-1	**B-2**	**B-3**	**B-4**	**B-5**	**B-6**	**B-7**	**B-8**
$\Delta E_{FM\text{-}AFM}$	1.140	0.340	0.840	0.400	0.700	0.320	0.340	0.250
μ_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**
$\Delta E_{FM\text{-}AFM}$	0.550	0.310	0.570	0.330	0.410	0.050	0.220	1.050
μ_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

[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.

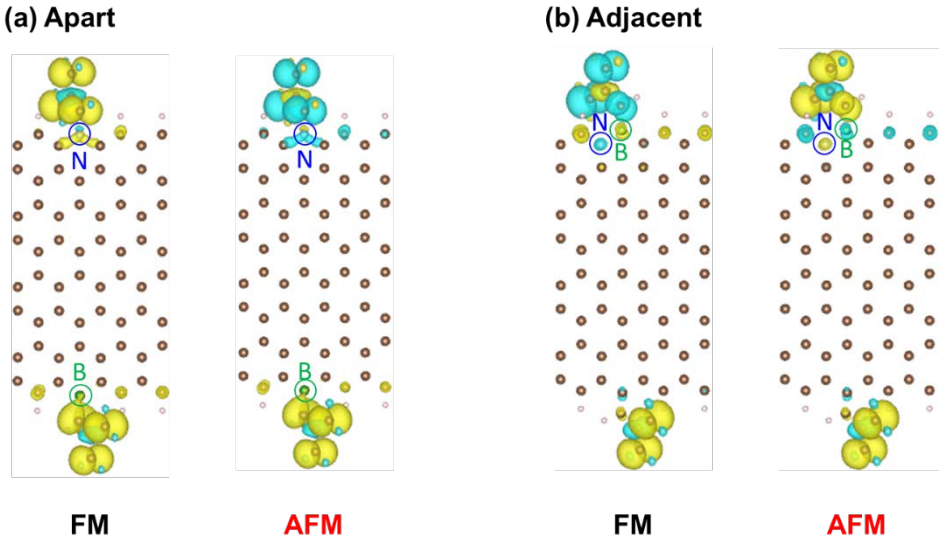


Figure S2. Comparison of magnetic ground state of BN-doped **TZT** system depending on the doping position of B and N atom. (a) B and N apart (b) B and N adjacent. Ground spin configuration were marked in red.

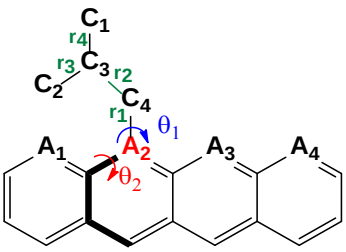
Table S3. Calculated Electronic Energy Difference between FM and AFM Magnetic Configurations ($\Delta E_{FM\text{-}AFM}$ in meV), Net Magnetic Moment per Unit Cell (μ_s in μ_B) of B- and N-Doped System for Doping Position. Calculated with PBE Functional

	undoped		**BN apart**		**BN adjacent**	
	FM	AFM	FM	AFM	FM	AFM
$\Delta E_{FM\text{-}AFM}$	0.330		0.280		0.800	
μ_s (μ_B)	1.964	0.001	3.951	0.040	2.082	0.116

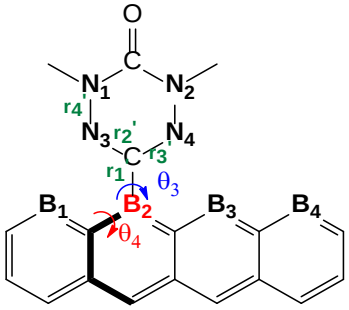
Table S4. Atomic Magnetizations ($\mu(X_i)$ where X = C, N, A, and B in $0.0001\mu_B$) on radical (C_n or N_n) and Edge Atoms (A_n or B_n) Compared to Undoped System by Doping (Atom Magnetizations of Undoped System were Written in Brackets: [C_n, N_n]) for TZO, Selected Bond Lengths (r1- r4 and r1'- r4' in Å), Dihedral Angle between TMM Radical and Ipso Atom against ZGNR Coupler (θ_1 - θ_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 side



OVER side



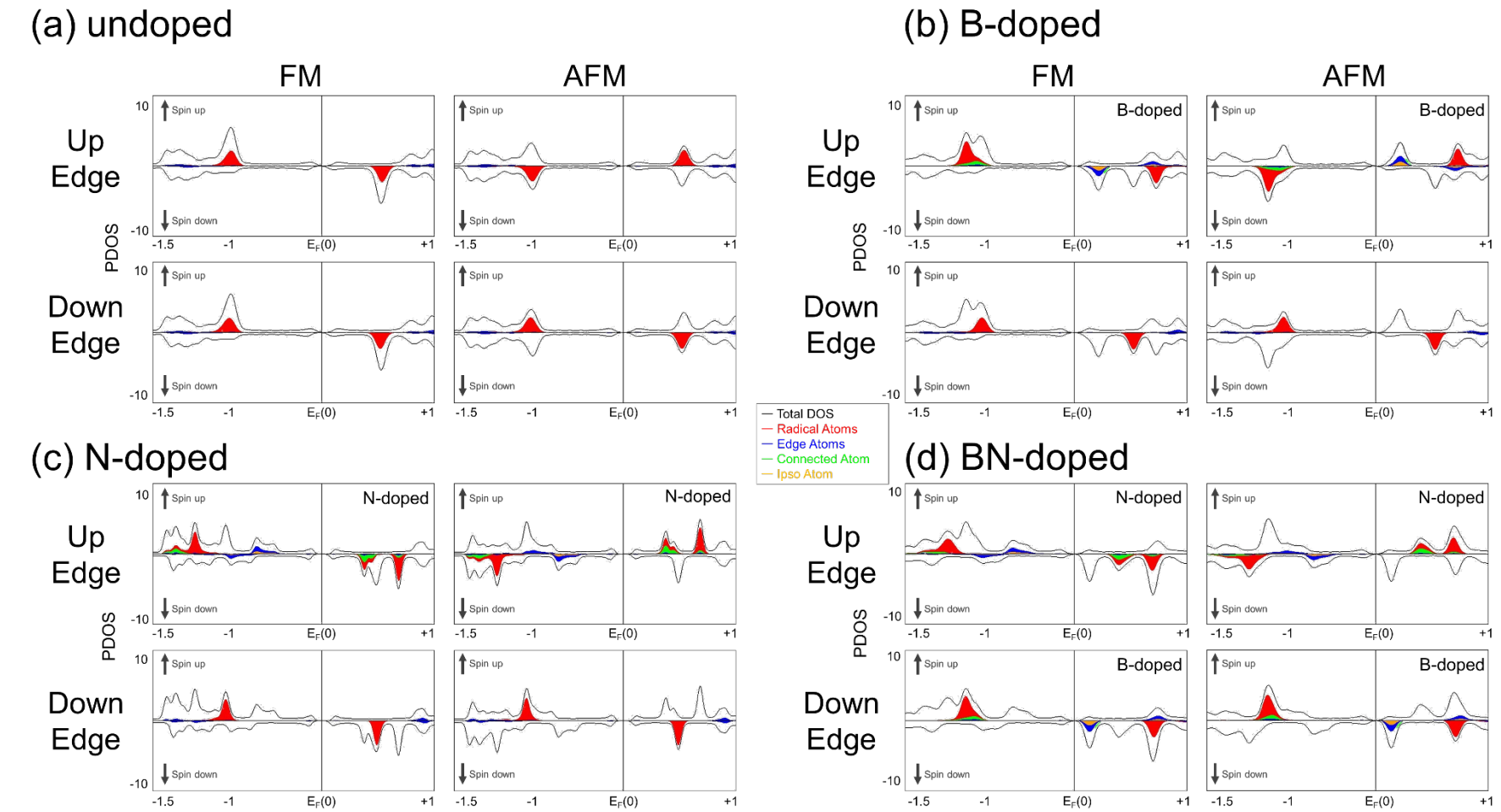


Figure S3. Density of States diagram for (a) undoped, (b) B-doped, (c) N-doped and (d) BN-doped **TZT** system. Each "Up edge" and "Down edge" includes both radical and edge atoms. Unfilled black line represents total DOS. Filled red, blue, green, and yellow represents DOS of total radical atoms, edge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

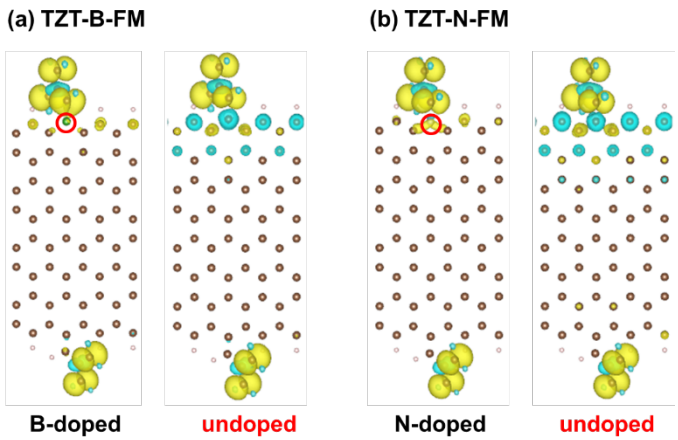


Figure S4. Spin distribution patterns of doped and undoped **TZT** system at B and N doped geometry obtained by PBE-vdW-DF calculations.

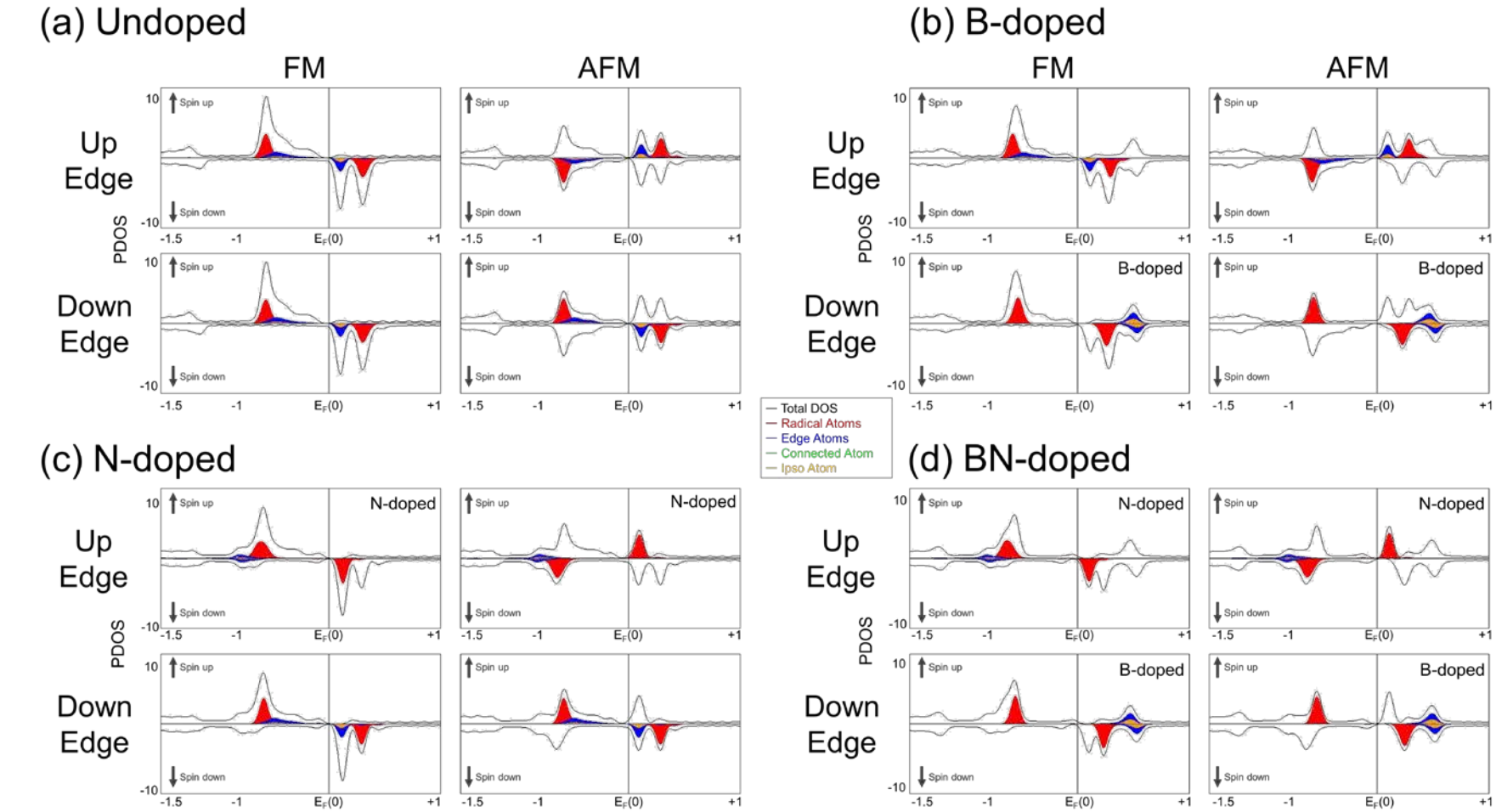


Figure S5. Density of States diagram for (a) undoped, (b) B-doped, (c) N-doped and (d) BN-doped **OZO** system. Each "Up edge" and "Down edge" includes both radical and edge atoms. Unfilled black line represents total DOS. Filled red, blue, green, and yellow represents DOS of total radical atoms, edge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

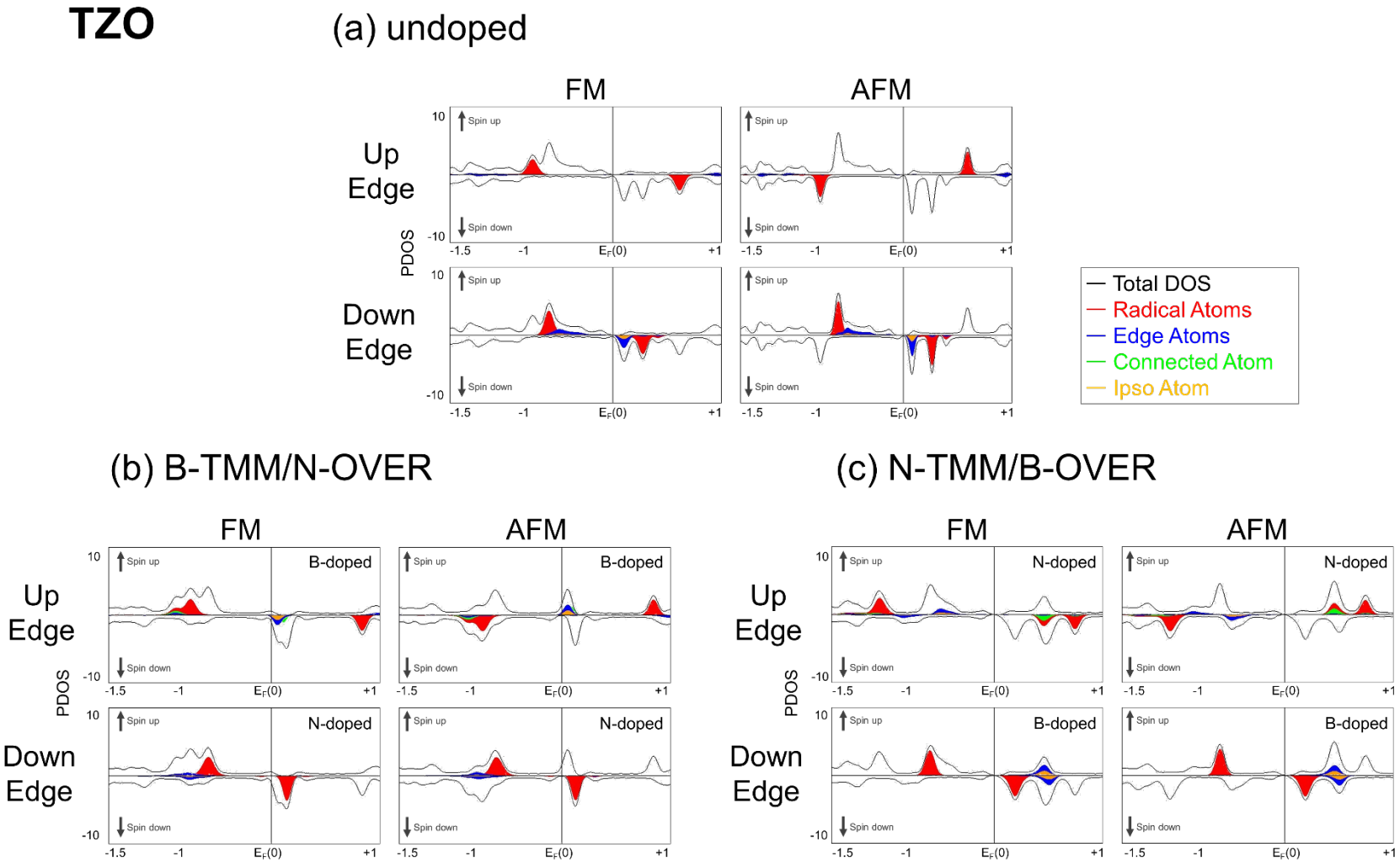


Figure S6. Density of States diagram for (a) undoped, (b) B-TMM/N-OVER, (c) N-TMM/B-OVER, (d) B-TMM, (e) B-OVER, (f) N-TMM, and (g) N-OVER **TZO** system. Each "Up edge" and "Down edge" includes both radical and edge atoms. Unfilled black line represents total DOS. Filled red, blue, green, and yellow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

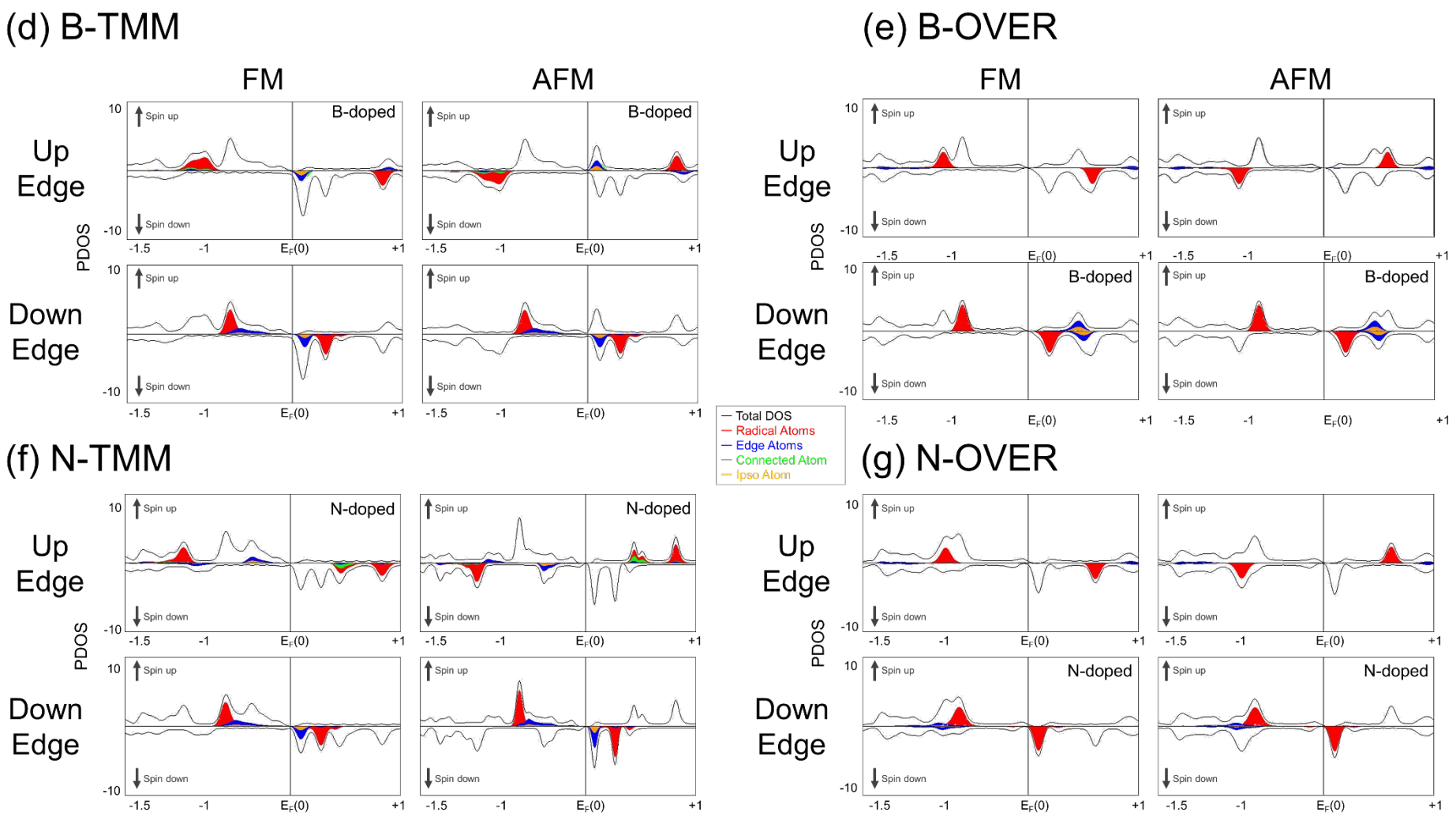


Figure S6. (Continued)