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

Electronic Supplementary Information

for

Electric Field Effect on the Magnetic Properties of Zigzag MoS_2 Nanoribbons with Different Edge Passivation

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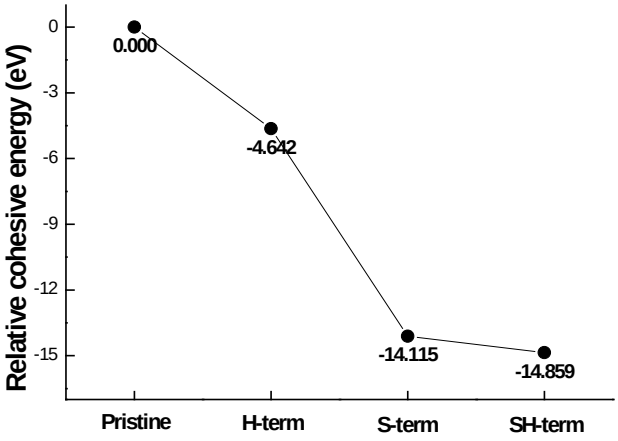

Fig. S1 Cohesive energy of **Pristine**, **H-term**, **S-term**, and **SH-term** relative to the electronic energy of **Pristine** system.

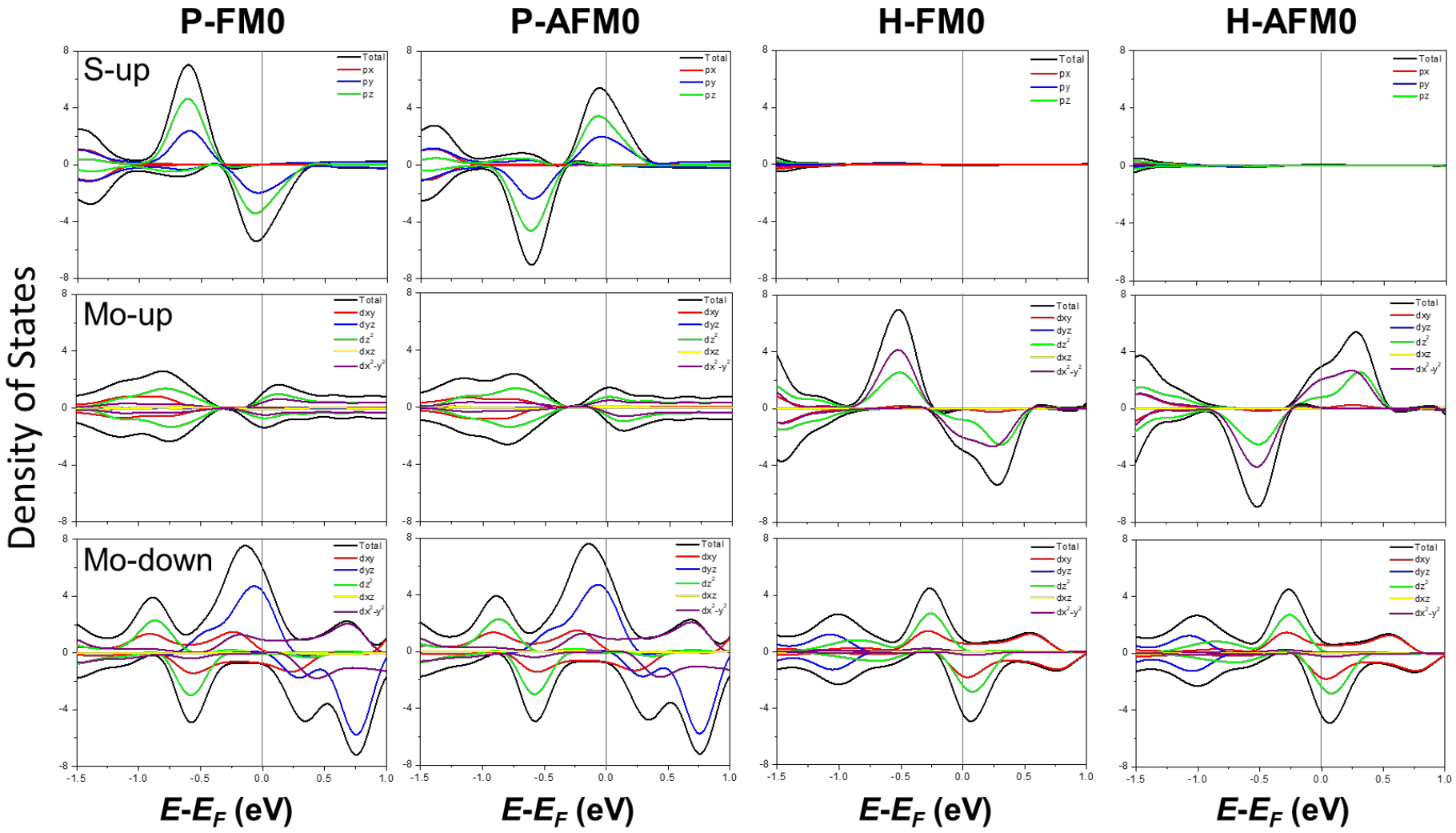

Fig. S2 Partial density of states (PDOS) of S-up, Mo-up, and Mo-down atoms of **P-FM0, P-AFM0, H-FM0**, and **H-AFM0**. For S-up atoms, black, red, blue, and green lines indicate PDOS of total, p_x, p_y, and p_z orbital, respectively. For Mo-up and Mo-down atoms, black, red, blue, green, yellow, and purple lines indicate PDOS of total, d_{xy}, d_{yz}, d_{z^2}, d_{xz}, and $d_{x^2-y^2}$ orbital, respectively.

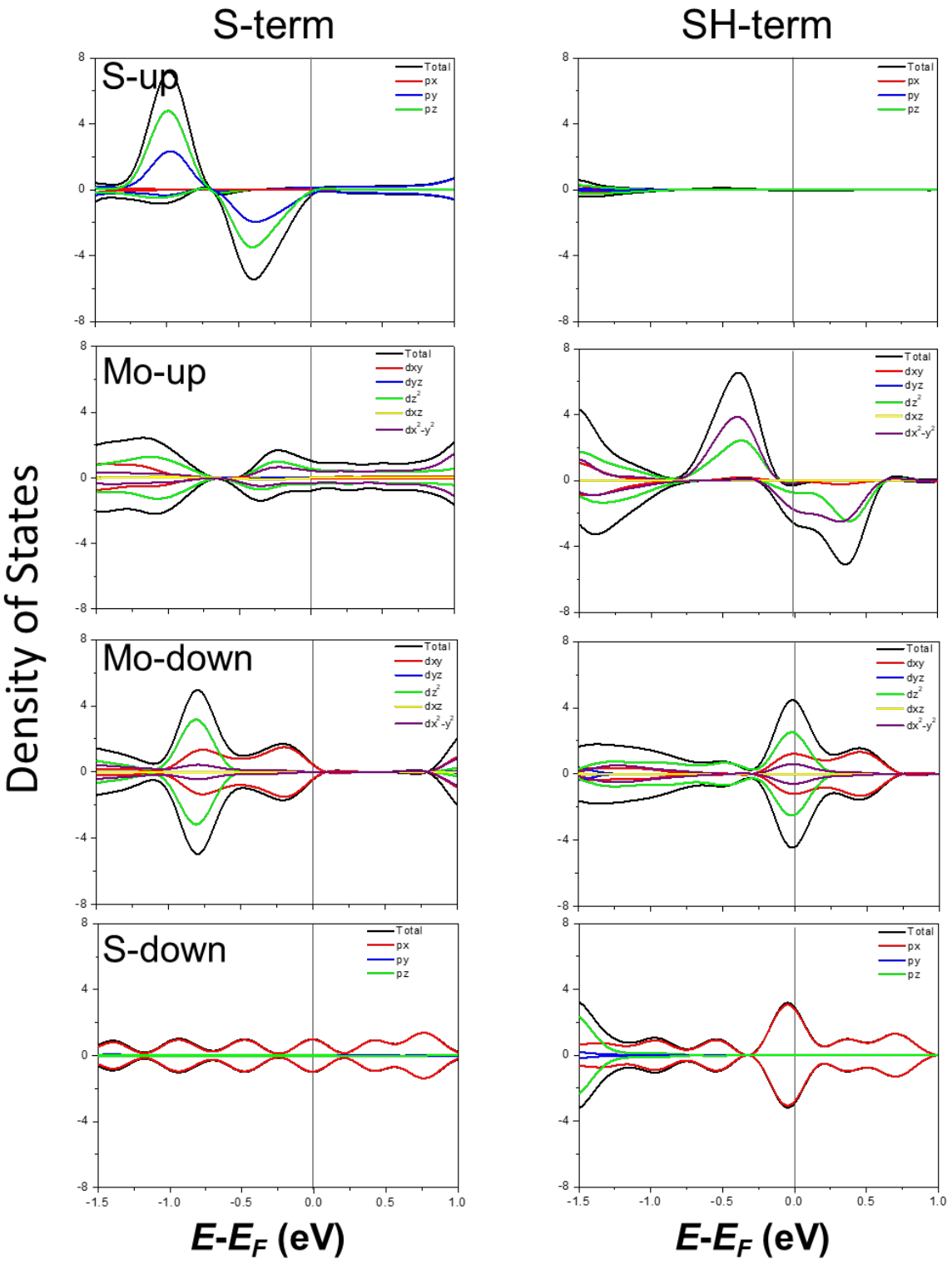

Fig. S3 Partial density of states (PDOS) of S-up, Mo-up, Mo-down, and S-down atoms of **S-term** and **SH-term**. For S-up and S-down atoms, black, red, blue, and green lines indicate PDOS of total, p_x, p_y, and p_z orbital, respectively. For Mo-up and Mo-down atoms, black, red, blue, green, yellow, and purple lines indicate pDOS of total, d_{xy}, d_{yz}, d_z^2, d_{xz}, and $d_{x^2-y^2}$ orbital, respectively.

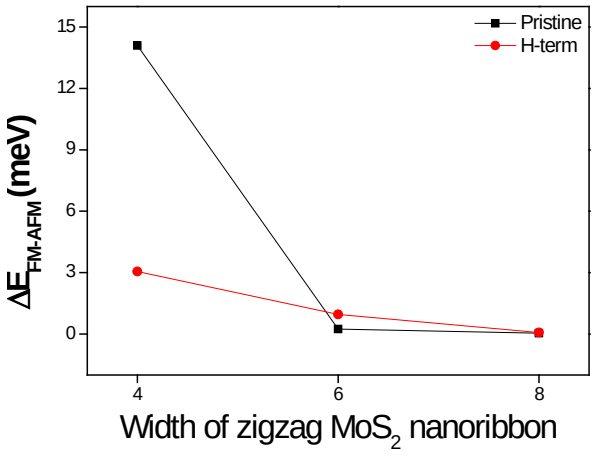

Fig. S4 Electronic energy difference between FM and AFM configuration (ΔE_{FM-AFM}) of **Pristine** and **H-term** by the width of nanoribbon.

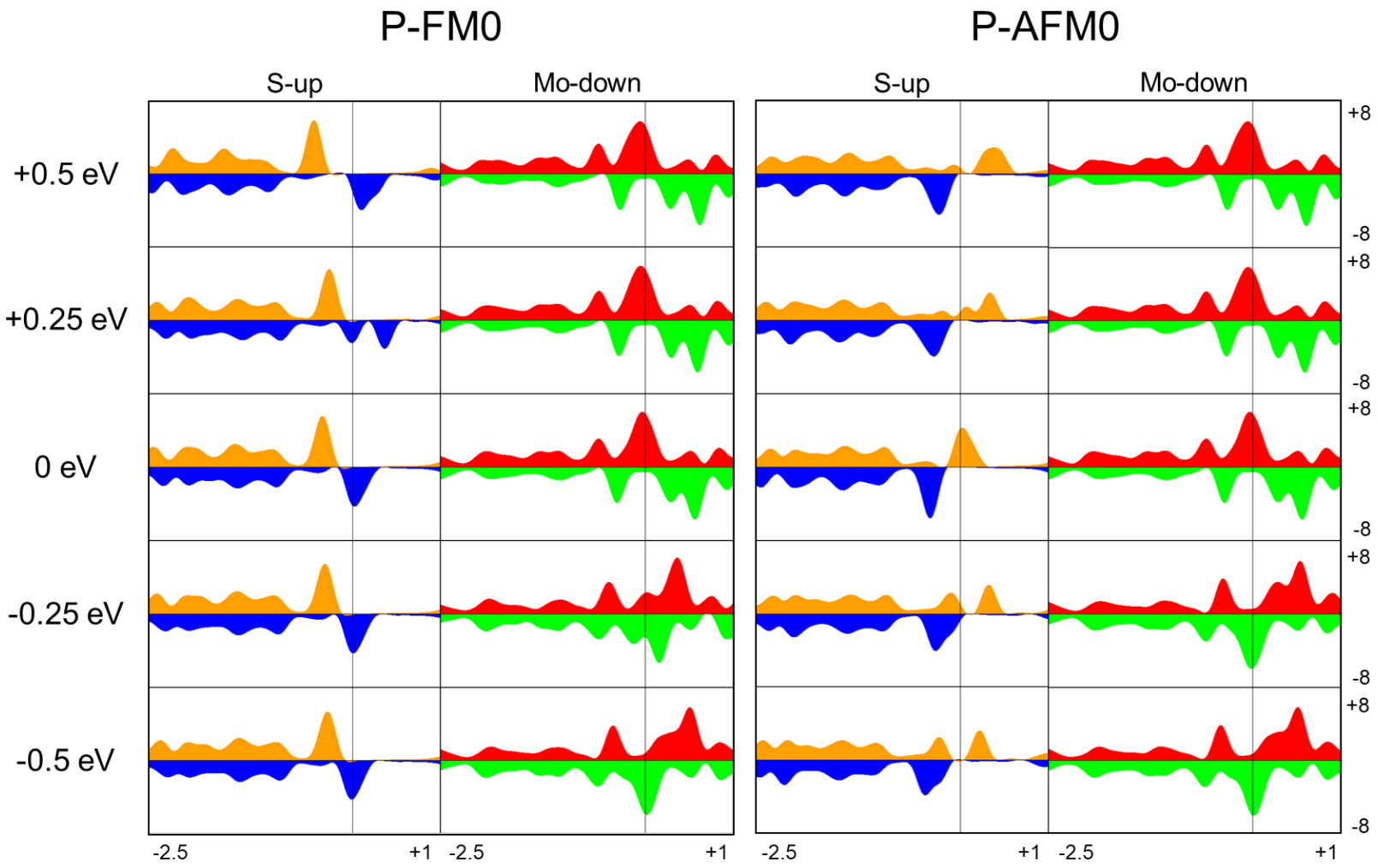

Fig. S5 Variation of total DOS of spin containing atoms by the strength of the applied electric field for **Pristine**, **H-term**, **S-term** and **SH-term**.

Yellow/blue, red/green color indicates the DOS of up/down spin electrons of S and Mo atoms, respectively.

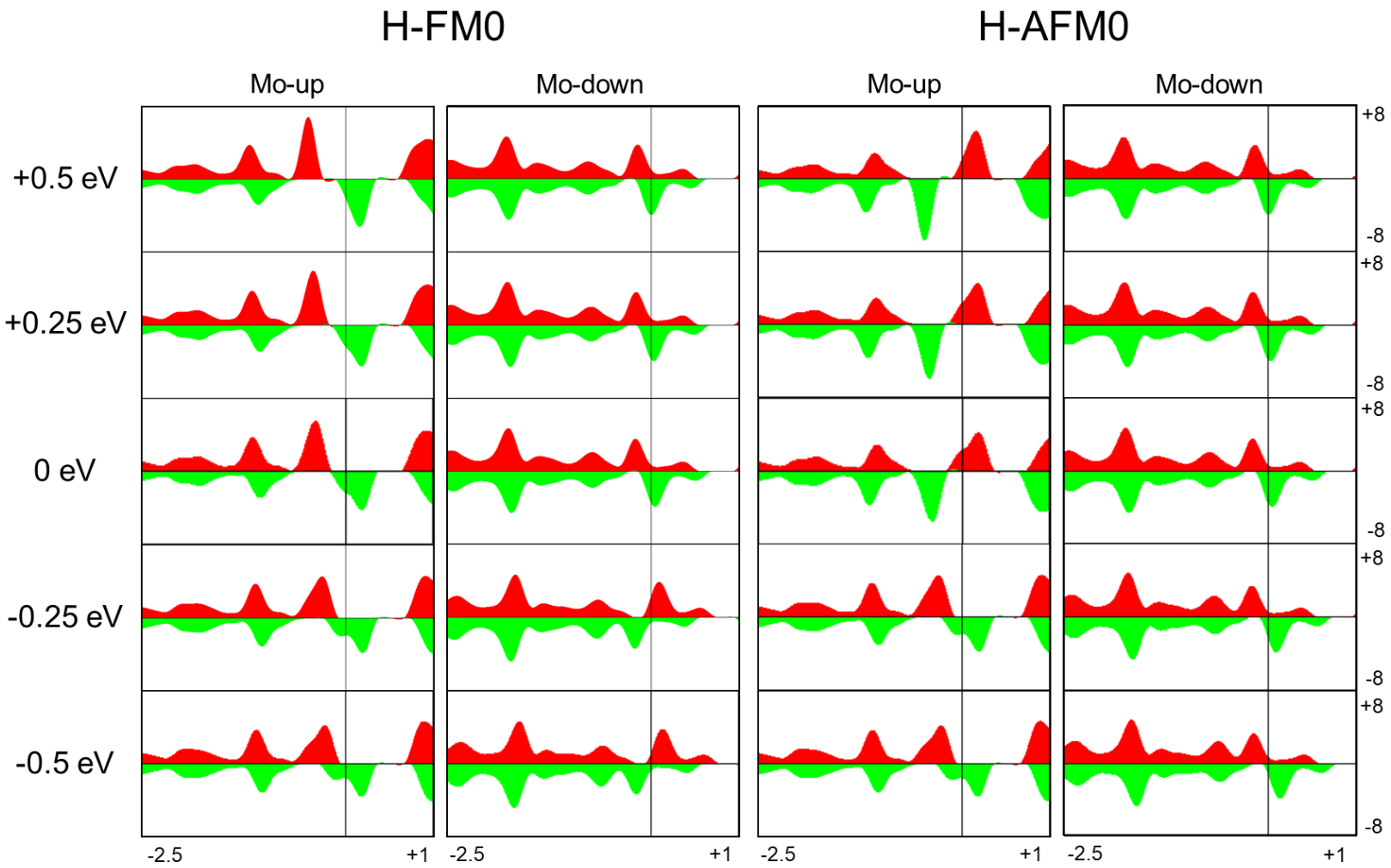

Fig. S5 (Continued)

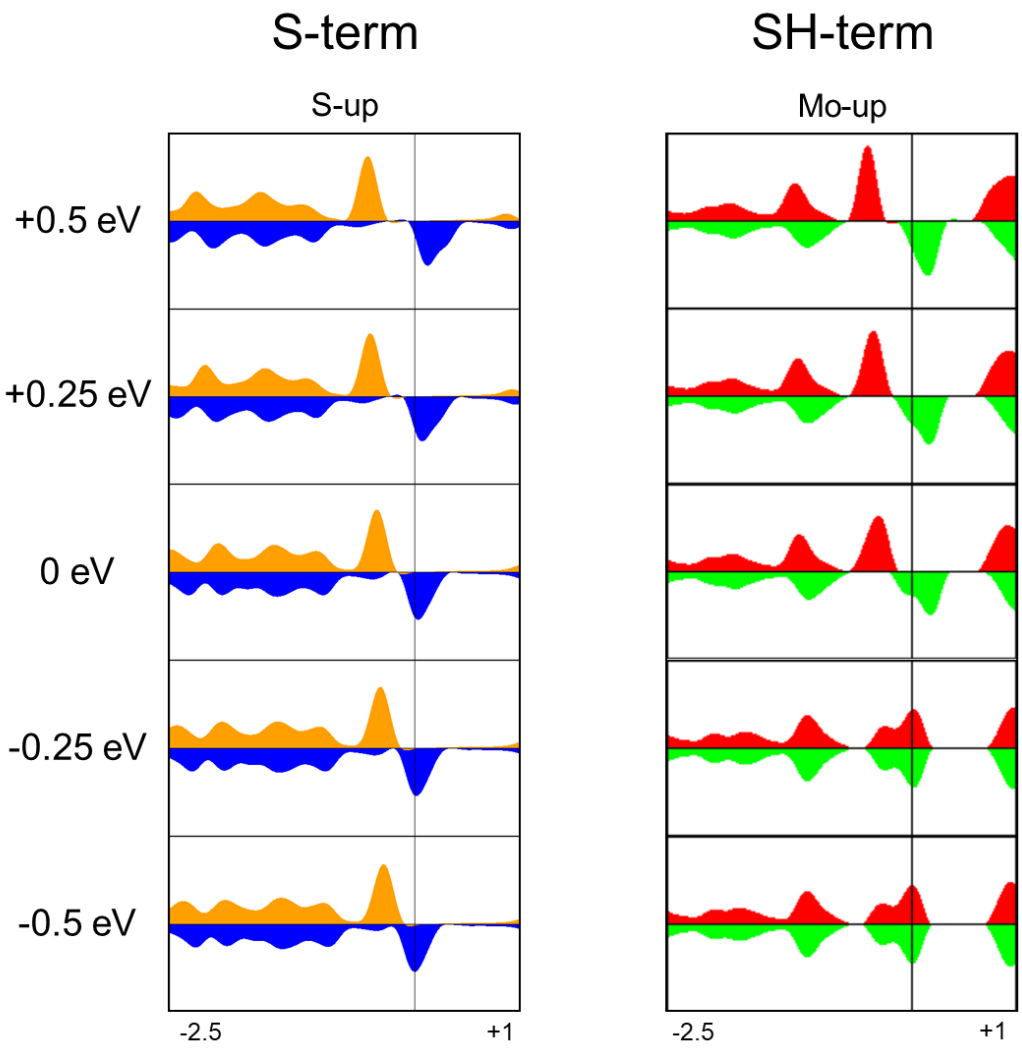

Fig. S5 (Continued)

Table S1 Variation of Total DOS of Edge Atoms Relative to Total DOS at 0 eV.

	P-FM								P-AFM							
F_{Ext}	-0.5		-0.25		+0.25		+0.5		-0.5		-0.25		+0.25		+0.5	
Spin	Up	Down	Up	Down	Up	Down	Up	Down	Up	Down	Up	Down	Up	Down	Up	Down
S-up	-6.57	11.94	-3.36	4.79	4.79	-2.89	16.27	-22.06	2.59	-9.66	6.97	-4.02	-11.40	0.18	-11.31	6.46
Mo-down	-125.74	89.17	-117.35	43.05	27.25	-2.04	54.24	-1.30	-124.67	95.16	-127.22	113.49	28.67	-1.06	47.16	-2.38
	H-FM								H-AFM							
Mo-up	-49.69	8.82	-33.85	7.22	14.34	-3.92	42.61	-11.55	121.82	-163.13	138.39	-165.15	-3.58	15.48	-11.56	42.63
Mo-down	-38.14	60.58	-41.38	50.79	-2.55	1.12	-7.50	6.11	20.60	1.53	11.14	-1.76	-3.33	1.50	-7.84	5.61
	S-term								SH-term							
S-up	-7.48	14.38	-4.11	7.51	9.55	-13.33	15.20	-19.48	13.76	4.86	20.01	11.08	-1.47	-1.25	-3.95	-4.05
Mo-up	4.28	4.43	1.86	1.87	-4.23	-3.01	-5.59	-5.06	-101.60	52.90	-100.38	55.12	27.71	-6.37	58.77	-13.83

Table S2 Variation of Partial DOS of Edge Atoms by Orbital Relative to PDOS at 0 eV, Changed by Strength of Electric Field. Rounded off from the First Decimal Point.

P-FM0								
	S-up			Mo-down				
F_{Ext}	p_x	p_y	p_z	d_{xy}	d_{yz}	d_{z^2}	d_{xz}	$d_{x^2-y^2}$
-0.5	1 / 1	3 / 4	-11 / 7	-16 / 18	-107 / 73	15 / -16	0 / 0	-17 / 14
-0.25	1 / 1	1 / 1	-5 / 3	-14 / 19	-98 / 20	12 / -13	0 / 0	-17 / 16
+0.25	-2 / -2	0 / 4	6 / -5	-1 / -1	27 / 0	0 / -1	0 / 0	1 / 0
+0.5	-3 / -4	-4 / -3	24 / -15	-1 / 0	53 / 0	1 / -1	0 / 0	1 / 0
P-AFM0								
	S-up			Mo-down				
F_{Ext}	p_x	p_y	p_z	d_{xy}	d_{yz}	d_{z^2}	d_{xz}	$d_{x^2-y^2}$
-0.5	-5 / -5	8 / -3	-1 / -2	-15 / 18	-107 / 79	16 / -15	0 / 0	-17 / 13
-0.25	-3 / -3	11 / 0	-1 / -1	-17 / 18	-107 / 94	15 / -15	0 / 0	-18 / 17
+0.25	-3 / -3	0 / -6	-9 / 9	-1 / 0	28 / 0	1 / 0	0 / 0	1 / 0
+0.5	-2 / -2	1 / -4	-11 / 13	-2 / -1	46 / 0	1 / -1	0 / 0	2 / 0
H-FM0								
	Mo-up					Mo-down				
F_{Ext}	d_{xy}	d_{yz}	d_{z^2}	d_{xz}	$d_{x^2-y^2}$	d_{xy}	d_{yz}	d_{z^2}	d_{xz}	$d_{x^2-y^2}$
-0.5	-1 / 0	0 / 0	-12 / 3	0 / -1	-36 / 7	-17 / 9	8 / 4	-52 / 39	1 / 0	21 / 9
-0.25	-1/ 0	0 / 0	-9 / 2	0 / 0	-25 / 6	-15 / 10	6 / 1	-50 / 39	1 / -1	16 / 2
+0.25	0 / 0	0 / 0	4 / -1	0 / 0	10 / -3	0 / 2	-1 / -1	1 / 4	0 / 0	-3 / -3
+0.5	1 / 0	0 / 0	13 / -2	-1 / -1	30 / -8	1 / 6	-3 / -3	2 / 14	0 / 0	-8 / -10
H-AFM0								
	Mo-up					Mo-down				
F_{Ext}	d_{xy}	d_{yz}	d_{z^2}	d_{xz}	$d_{x^2-y^2}$	d_{xy}	d_{yz}	d_{z^2}	d_{xz}	$d_{x^2-y^2}$
-0.5	0 / -2	0 / 0	43 / -53	-2 / 1	80 / -108	-1 / -7	6 / 6	-2 / -11	0 / 0	17 / 13
-0.25	1 / -2	0 / 0	47 / -54	-1 / 1	92 / -111	-1 / -5	3 / 3	-1 / -9	0 / 0	9 / 8
+0.25	0 / 0	0 / 0	-1 / 5	-1 / -1	-2 / 11	0 / 2	-1 / -1	1 / 4	0 / 0	-3 / -4
+0.5	0 / 1	0 / 0	-2 / 13	-1 / -1	-8 / 30	1 / 6	-3 / -3	3 / 14	0 / 0	-8 / -10
	S-term					SH-term				

	S-up			Mo-up				
F_{Ext}	p_x	p_y	p_z	d_{xy}	d_{yz}	d_z^2	d_{xz}	$d_{x^2-y^2}$
-0.5	1 / 1	3 / 4	-12 / 9	-2 / 0	0 / 0	-35 / 17	4 / 2	-69 / -69
-0.25	1 / 1	1 / 2	-6 / 5	-1 / 1	0 / 0	-36 / 16	6 / 5	-69 / 34
+0.25	-2 / -2	-4 / -2	15 / -9	1 / 0	0 / 0	9 / -1	-1 / 0	19 / -5
+0.5	-3 / -3	-5 / -2	23 / -14	2 / 1	0 / 0	19 / -3	-2 / 1	40 / -11

Table S3 Bader Charge of Spin Containing Atoms of Pristine, H-term, S-term, and SH-term.

F_{EXT}		-0.5				-0.25				0				+0.25				+0.5			
P-FM0	S-up	-0.795	-0.634	-0.795	-0.636	-0.757	-0.615	-0.756	-0.614	-0.626	-0.626	-0.625	-0.626	-0.572	-0.600	-0.569	-0.698	-0.551	-0.553	-0.549	-0.653
	Mo-down	1.410	1.408	1.406	1.408	1.378	1.379	1.379	1.378	1.355	1.355	1.355	1.355	1.312	1.312	1.312	1.313	1.284	1.283	1.283	1.283
P-AFM0	S-up	-0.688	-0.688	-0.688	-0.688	-0.655	-0.654	-0.657	-0.654	-0.626	-0.626	-0.626	-0.626	-0.574	-0.658	-0.574	-0.658	-0.545	-0.547	-0.547	-0.547
	Mo-down	1.399	1.399	1.399	1.399	1.377	1.377	1.376	1.377	1.355	1.355	1.355	1.355	1.316	1.316	1.316	1.316	1.280	1.281	1.280	1.280
H-FM0	Mo-up	1.641	1.645	1.646	1.639	1.646	1.647	1.646	1.645	1.649	1.652	1.652	1.648	1.669	1.673	1.671	1.669	1.670	1.670	1.670	1.670
	Mo-down	1.647	1.646	1.646	1.646	1.648	1.649	1.648	1.648	1.649	1.652	1.652	1.649	1.664	1.663	1.662	1.663	1.665	1.666	1.665	1.665
H-AFM0	Mo-up	1.930	1.930	1.930	1.930	1.924	1.924	1.924	1.924	1.922	1.922	1.922	1.921	1.903	1.899	1.900	1.900	1.898	1.896	1.898	1.898
	Mo-down	1.932	1.930	1.930	1.930	1.922	1.923	1.923	1.923	1.923	1.922	1.922	1.921	1.909	1.910	1.909	1.910	1.897	1.900	1.900	1.898
S-term	S-up	-0.683	-0.689	-0.681	-0.681	-0.649	-0.648	-0.657	-0.647	-0.624	-0.624	-0.624	-0.624	-0.563	-0.585	-0.564	-0.569	-0.556	-0.563	-0.517	-0.522
SH-term	Mo-up	1.570	1.570	1.570	1.570	1.582	1.582	1.582	1.582	1577	1577	1577	1577	1590	1590	1590	1590	1600	1600	1600	1600

Table S4 Average Bader Charge Difference between FM and AFM Configuration for Each Edge Atoms

	Pristine					H-term				
F_{Ext}	-0.5	-0.25	0	+0.25	+0.5	-0.5	-0.25	0	+0.25	+0.5
$\Delta\sigma_{S\text{-}up}$	0.080	0.070	0.000	0.026	0.030	0.007	0.006	0.004	0.007	0.007
$\Delta\sigma_{Mo\text{-}up}$	0.070	0.071	0.000	0.012	0.048	0.003	0.002	0.000	0.008	0.005
$\Delta\sigma_{Mo\text{-}down}$	0.009	0.002	0.000	0.004	0.003	0.001	0.001	0.000	0.009	0.002
Sum	0.160	0.143	0.001	0.042	0.082	0.011	0.009	0.004	0.023	0.014

Table S5 Average Magnetization Difference between FM and AFM Configuration for Each Edge Atoms.

	Pristine					H-term				
F_{Ext}	-0.5	-0.25	0	+0.25	+0.5	-0.5	-0.25	0	+0.25	+0.5
$\Delta\rho_{S\text{-}up}$	0.152	0.142	0.001	0.061	0.062	0.000	0.000	0.000	0.000	0.000
$\Delta\rho_{Mo\text{-}up}$	0.031	0.048	0.000	0.021	0.076	0.003	0.003	0.001	0.003	0.001
$\Delta\rho_{Mo\text{-}down}$	0.020	0.337	0.001	0.001	0.016	0.000	0.001	0.000	0.002	0.002
Sum	0.203	0.526	0.002	0.082	0.154	0.003	0.004	0.001	0.005	0.003