Electronic Supplementary Information for

Article

Two-Dimensional $VSi_2X_2N_2$ (X = P, As, Sb, Bi) Janus Monolayers: Spin-Polarized Electronic Structure and Perpendicular Magnetic Anisotropy

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Table S1. The bond lengths and bond angles of $VSi_2X_2N_2$ (X = N, P, As, Sb, Bi).

		$VSi_2P_2N_2$	$VSi_2As_2N_2$	$VSi_2Sb_2N_2$	$VSi_2Bi_2N_2$
Bond length (Å)	X2-Si2	2.16	2.35	2.99	3.18
	Si2-X1	2.20	3.87	3.23	3.24
	X1-V	2.35	2.47	2.88	2.96
	V-N1	3.70	2.02	2.01	2.01
	N1-Si1	3.55	3.54	3.49	3.55
	Si1-N2	1.84	1.83	1.80	1.83
Bond angle (°)	X2-Si2-X1	109.22	113.34	144.42	146.04
	Si2-X1-V	80.97	85.65	142.89	143.14
	X1-V-N1	69.88	72.32	131.54	129.77
	V-N1-Si1	65.45	64.80	67.02	64.46
	N1-Si1-N2	52.54	52.75	53.96	52.71

Table S2. Atomic coordinates of the optimized structure of $VSi_2P_2N_2$ monolayer.

	x	*y*	*z*
P_1	0.6666686270878315	0.3333314399121705	0.5050739936883875
P_2	0.3333332664599762	0.6666667125400253	0.6268130177652153
N_1	0.6666685309369211	0.3333315360630808	0.4152721547705426
N_2	0.3333336145708446	0.6666663644291574	0.3368278792805816
V	0.0000022097204372	0.0000022097204372	0.4506716777719242
Si_1	0.6666670065202032	0.3333330604797989	0.3528557464600939
Si_2	0.6666669687037831	0.3333330982962189	0.5831755382632576

Table S3. Atomic coordinates of the optimized structure of $VSi_2As_2N_2$ monolayer.

	x	*y*	*z*
As_1	0.6666838020279595	0.3333162649720427	0.5036813742146935
As_2	0.3333298306667071	0.6666701483332945	0.6359709330855509
N_1	0.6666699557446215	0.3333301112553805	0.4125484532768726
N_2	0.3333310736712318	0.6666689053287700	0.3370464565196497
V	0.0000051213847297	0.9999948786152707	0.4452831621051264
Si_1	0.6666664144019874	0.3333336525980146	0.3525682911159234
Si_2	0.6666540261027670	0.3333460408972350	0.5835913376821853

Table S4. Atomic coordinates of the optimized structure of $VSi_2Sb_2N_2$ monolayer.

	x	*y*	*z*
Sb_1	0.6666665795485410	0.3333334874514615	0.5019840731830711
Sb_2	0.3333314222492834	0.6666685567507163	0.6892654170201415
N_1	0.6666651360755185	0.3333349309244868	0.3922846590070920
N_2	0.3333363634950714	0.6666636155049300	0.3183268055502706
V	0.9999969858501212	0.0000030141498768	0.4259442984796729
Si_1	0.6666698201841047	0.3333302468158973	0.3340237055614083
Si_2	0.6666739165973508	0.3333261504026514	0.6088610491983447

Table S5. Atomic coordinates of the optimized structure of $VSi_2Bi_2N_2$ monolayer.

	x	*y*	*z*
Bi_1	0.6666689344962563	0.3333311325037456	0.4975510481970475
Bi_2	0.3333349980017413	0.6666649809982603	0.6719813870948577
N_1	0.6666684330050422	0.3333316339949601	0.3993499815496128
N_2	0.3333348908478208	0.6666650881521807	0.3336806094294349
V	0.0000017935703357	0.9999982064296640	0.4272726582631327
Si_1	0.6666682123142769	0.3333318546857253	0.3470602717747436
Si_2	0.6666629617645241	0.3333371052354782	0.5937940516911737

Table S6. The charge transfer of each atom of $VSi_2X_2N_2$ monolayer.

	Δq_{X1}(e)	Δq_{N1}(e)	Δq_{N2}(e)	Δq_{X2}(e)	Δq_{V}(e)	Δq_{Si1}(e)	Δq_{Si2}(e)
$VSi_2P_2N_2$	-0.6343	0.0706	-0.0828	-0.8388	0.2754	0.1029	1.107
$VSi_2As_2N_2$	-0.9446	0.0902	-0.0736	-1.7252	0.3289	0.0954	2.2289
$VSi_2Sb_2N_2$	-1.2663	0.07	-0.0431	-2.2374	0.434	0.068	2.9747
$VSi_2Bi_2N_2$	-1.3339	0.1043	-0.0757	-2.2748	0.4313	0.1137	3.035

Table S7. The lattice constants (a=b), magnetic moment (M) and MAE of VSi_2X_2 (X=P, As, Sb, Bi).

	a=b (Å)	M (μ_B)
VSi_2P_2	3.27	1.28
VSi_2As_2	3.49	/
VSi_2Sb_2	3.11	1.42
VSi_2Bi_2	3.25	/

Table S8. The bond lengths (Å) and bond angle (°) of $VSi_2Sb_2N_2$ under different electric field.

	V-Sb	V-N	Sb1-Si1	Sb2-Si2	Sb-V-N
-0.6	2.881	2.015	3.279	2.984	131.536/86.226
-0.4	2.869	2.022	3.172	3.017	130.324/84.672
-0.2	2.881	2.015	3.248	2.987	131.524/86.212
0	2.881	2.014	3.230	2.988	131.536/86.234
+0.2	2.870	2.020	3.153	3.021	130.231/84.619
+0.4	2.881	2.014	3.218	2.988	131.530/86.219
+0.6	2.880	2.013	3.213	2.992	131.460/86.145

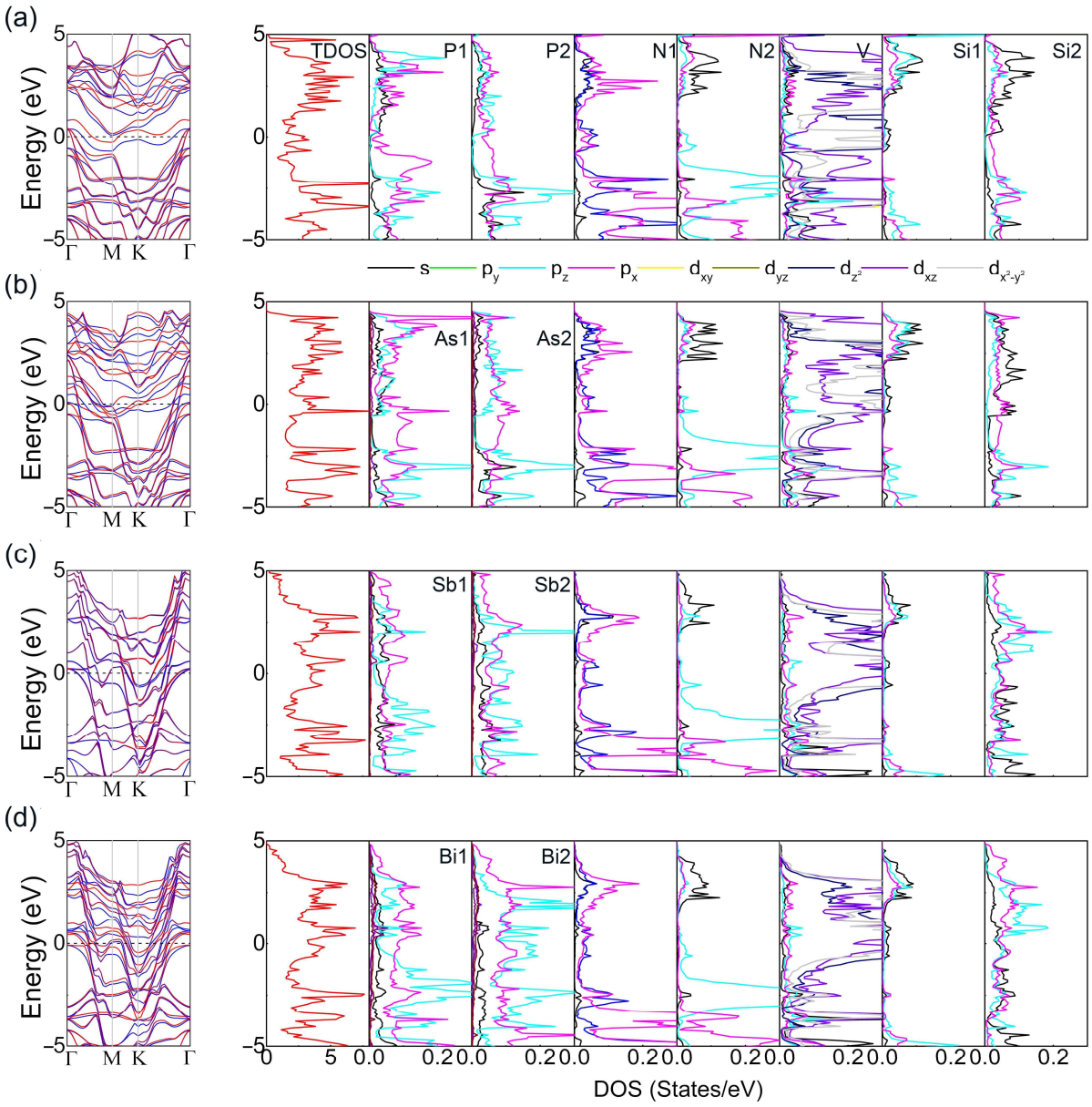

Figure S1. The band structure and density of states of (**a**) $VSi_2P_2N_2$, (**b**) $VSi_2As_2N_2$, (**c**) $VSi_2Sb_2N_2$, (**d**) $VSi_2Bi_2N_2$ with SOC. The Fermi level is set to zero.

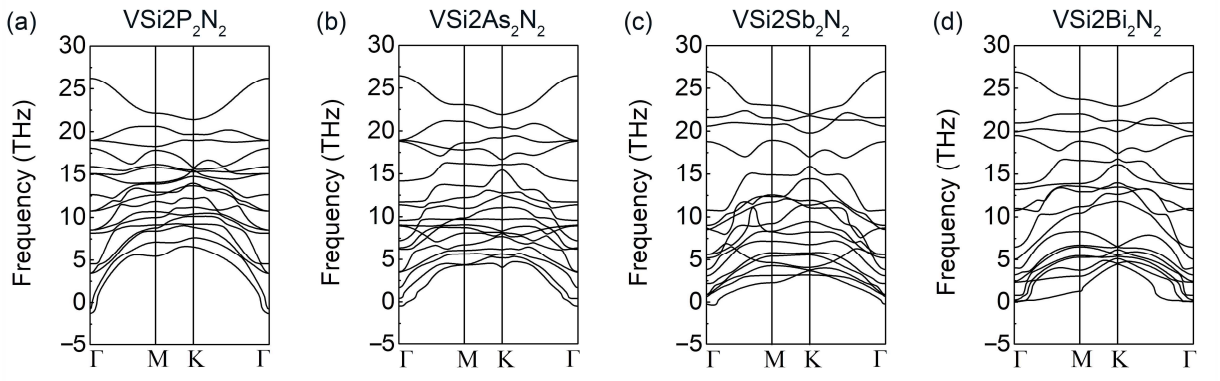

Figure S2. Phonon spectrum of the (**a-d**) $VSi_2X_2N_2$ monolayer.

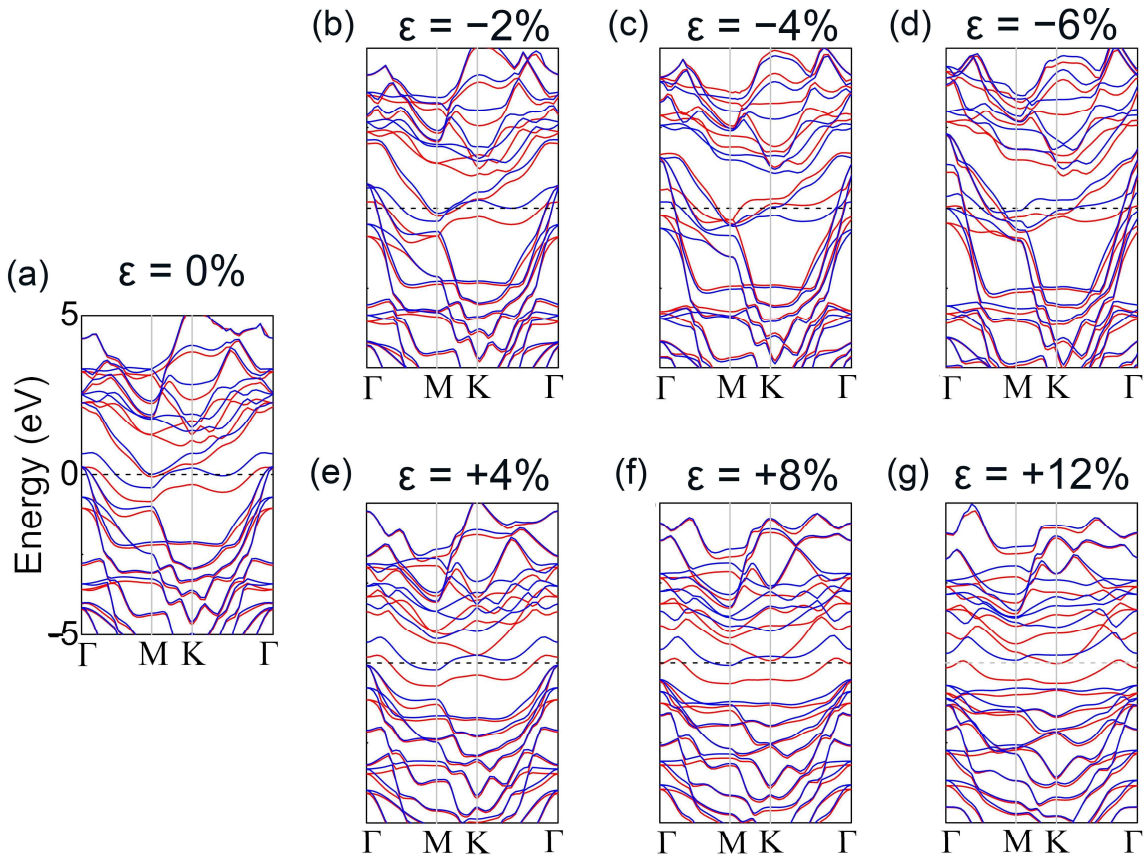

Figure S3. The band structure of $VSi_2P_2N_2$ under different biaxial strain. Red and blue lines in (**a**-**g**) represent the spin-up and spin-down band.

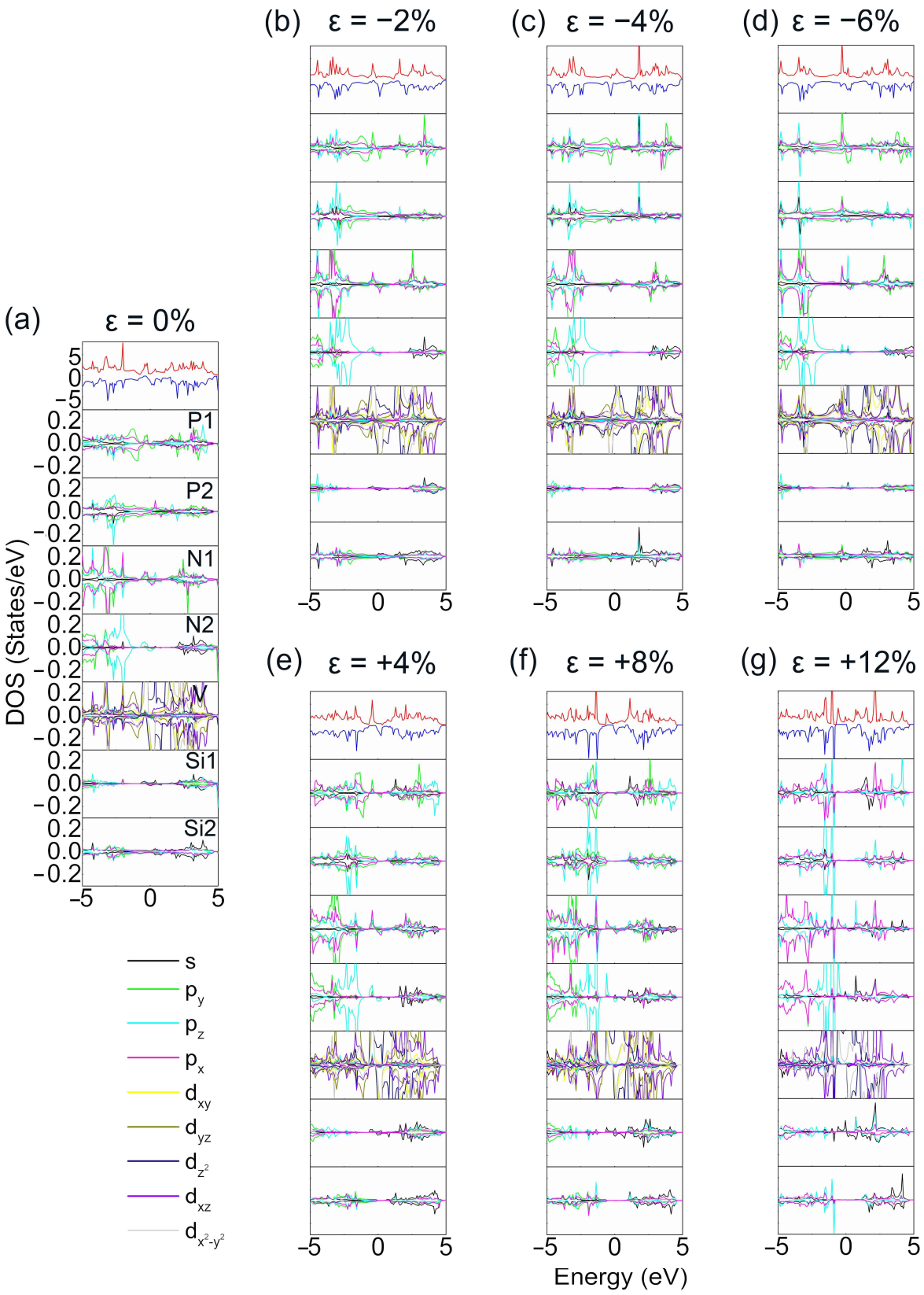

Figure S4. The density of states of (**a-g**) $VSi_2P_2N_2$ under different biaxial strain.

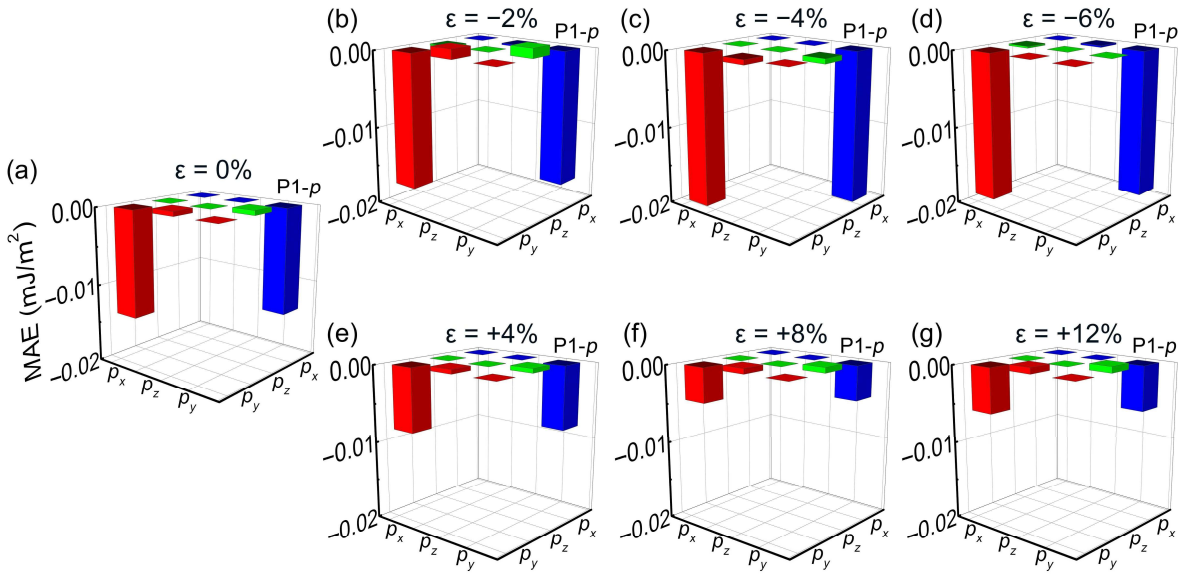

Figure S5. (**a**)-(**g**) Orbital-resolved MAE of P1-*p* orbitals in $VSi_2P_2N_2$ at different in-plane biaxial strains.

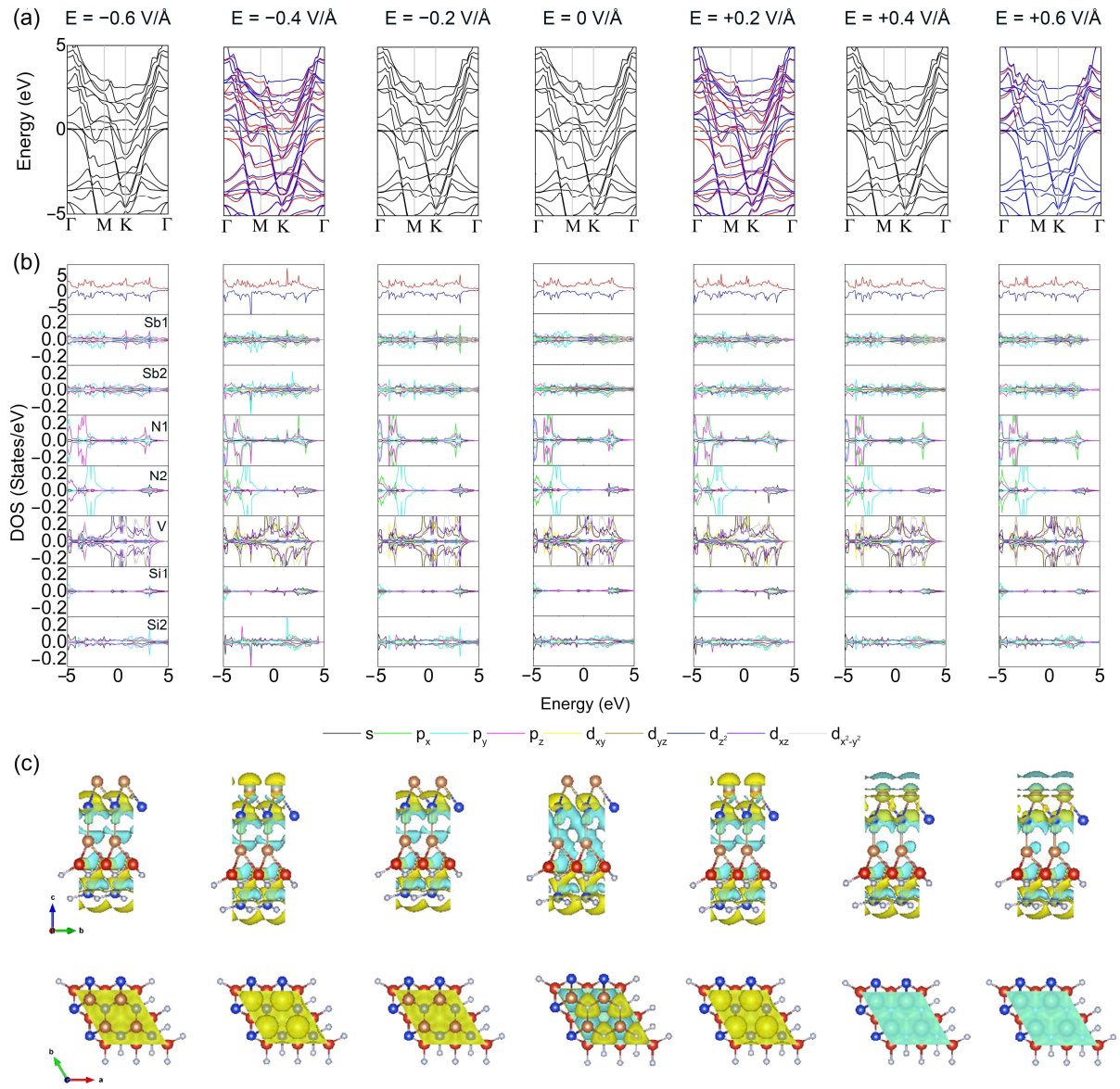

Figure S6. The band structure (**a**) and DOS (**b**) of $VSi_2Sb_2N_2$ with different external electric field. The red and blue represent the spin-up and spin-down channels, respectively, (**c**) charge density difference of $VSi_2Sb_2N_2$ with different external electric field.