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Defect effects on the electronic, valley, and magnetic properties of two-dimensional ferrovalley material VSi_2N_4

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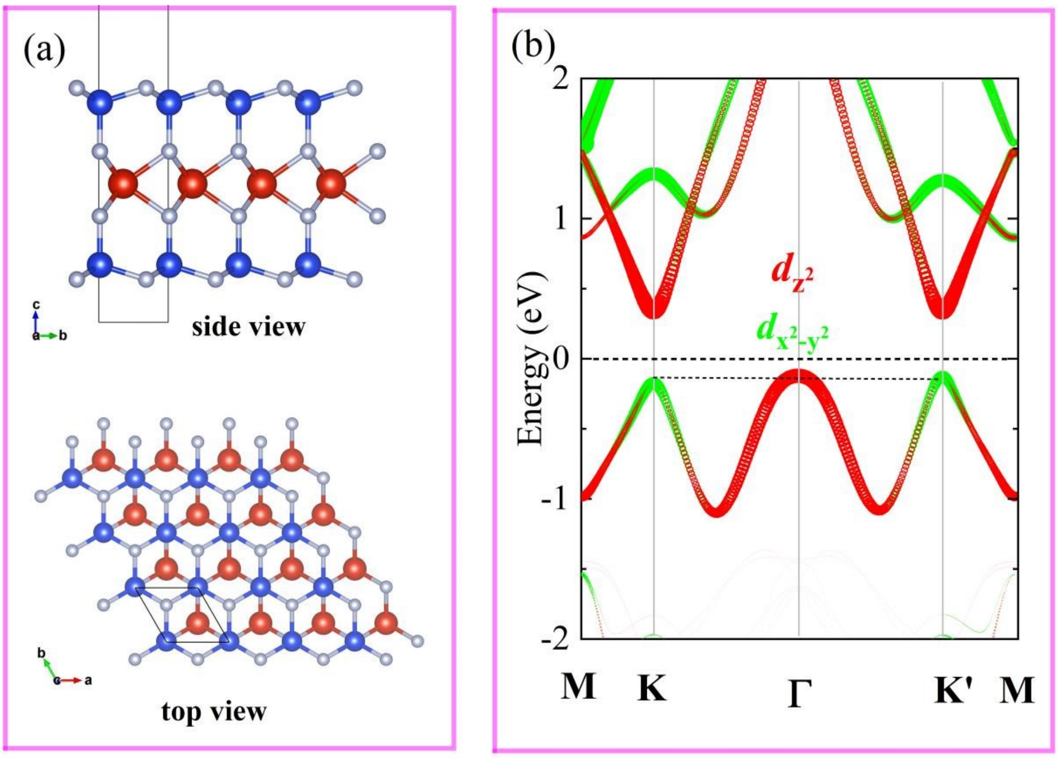

FIG. S1 (a) Lattice structure of VSi_2N_4, in which the gray, blue, and red balls denote N, Si, and V atoms, respectively. (b) Orbital projected band structure of the pristine VSi_2N_4. The Fermi level is set at the zero energy.

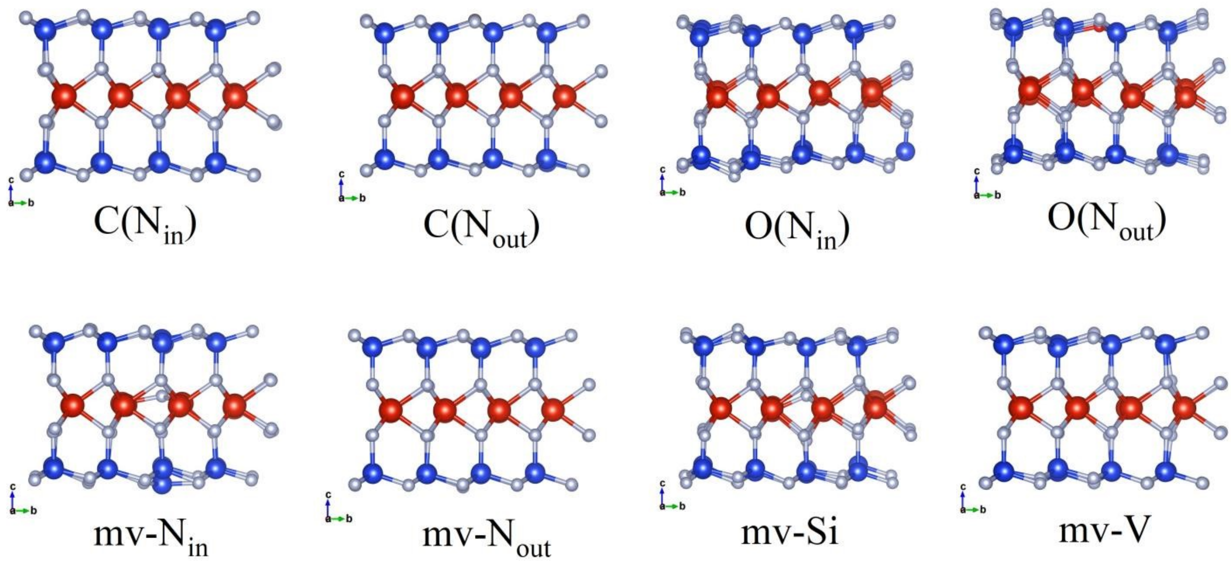

FIG. S2 The crystal structures of the defective VSi_2N_4 after AIMD. The gray, blue, and red balls denote N, Si, and V atoms, respectively.

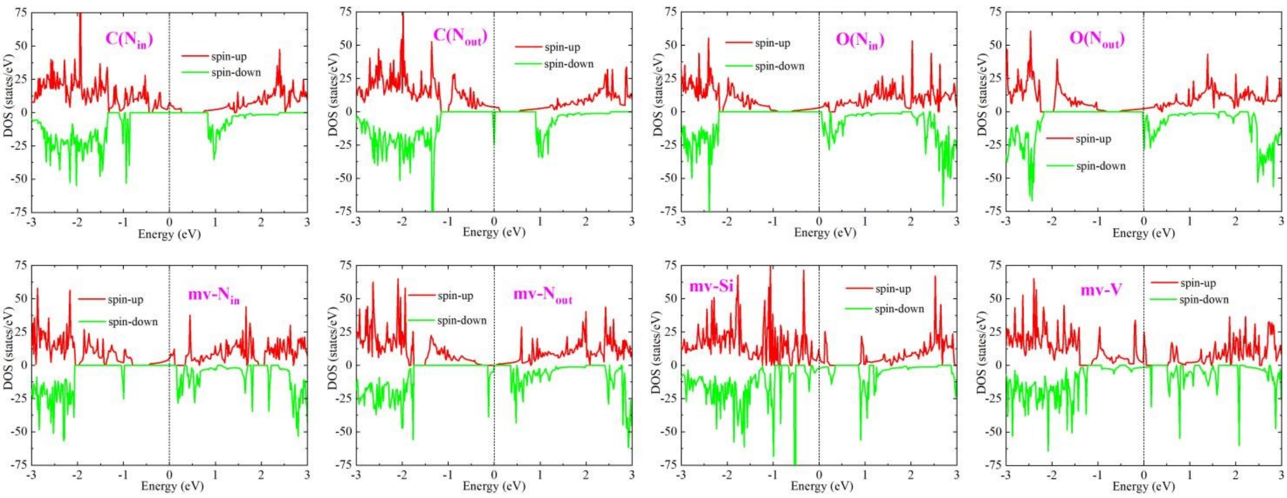

FIG. S3 The spin-polarized density of states of the doped and defected VSi_2N_4 with 3×3×1 supercell. The red and green lines denote the spin-up and spin-down channels, respectively, and the Fermi level is set at zero energy.

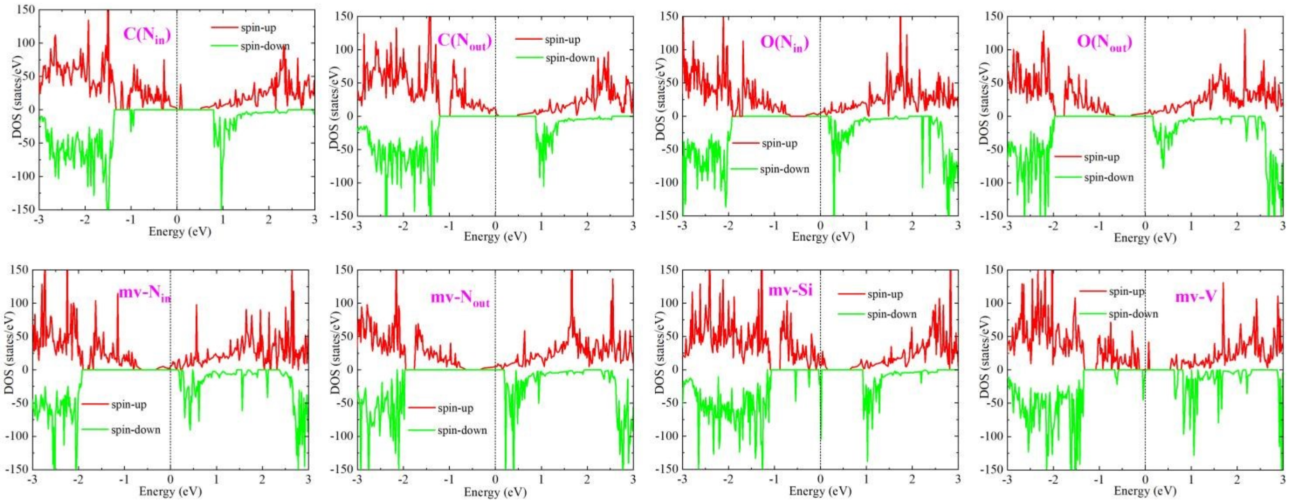

FIG. S4 The spin-polarized density of states of the doped and defected VSi_2N_4 with 5×5×1 supercell. The red and green lines denote the spin-up and spin-down channels, respectively, and the Fermi level is set at zero energy.

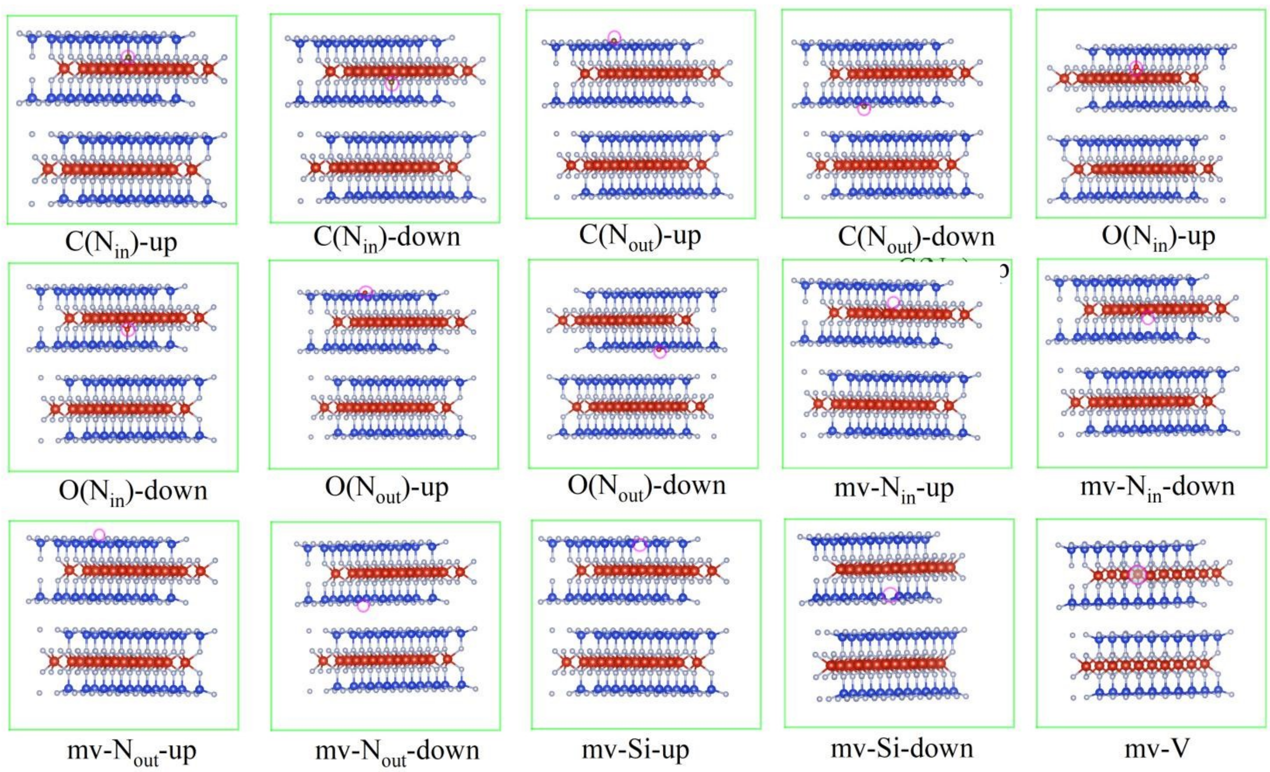

FIG. S5 Optimized structures of the defective VSi_2N_4 bilayers with AB-stacking. The gray, blue, and red balls denote N, Si, and V atoms, respectively. The defects have been marked by the pink circle.

TABLE SI. Using GGA+*U* method, the calculated magnetic quantities of the defective VSi_2N_4 using 3×3×1 supercell: total magnetic moment M_{total}, magnetic moment per V atom $M_{total/V}$, average magnetic moment of V surrounding defect (for the defective systems, M_V is calculated from the average of the neighboring V atoms) M_V, magnetic anisotropy energy E_{MAE}, and magnetic energy per V atom E_M.

	M_{total}(μ_B)	$M_{total/V}$(μ_B/V)	M_V(μ_B)	E_{MAE}(μeV/V)	E_M(meV/V)
VSi_2N_4	9.00	1.00	1.06	-33.3	282.5
C(N_{in})	8.00	0.89	0.81	-15.6	242.1
C(N_{out})	9.15	1.02	1.01	-9.7	250.2
O(N_{in})	9.99	1.11	1.14	-56.1	226.5
O(N_{out})	9.42	1.05	1.10	-41.5	218.5
Mv-N_{in}	10.00	1.11	1.25	-19.5	206.8
mv-N_{out}	8.03	0.89	0.67	-20.1	222.5
mv-Si	7.85	0.87	0.59	-1.3	171.3
mv-V	6.45	0.81	0.58	10.4	91.7

TABLE SII. Using GGA+U method, the calculated magnetic quantities of the defective VSi_2N_4 using 5×5×1 supercell: total magnetic moment M_{total}, magnetic moment per V atom $M_{total/V}$, average magnetic moment of V surrounding defect (for the defective systems, M_V is calculated from the average of the neighboring V atoms) M_V, magnetic anisotropy energy E_{MAE}, and magnetic energy per V atom E_M.

	M_{total}(μ_B)	$M_{total/V}$(μ_B/V)	M_V(μ_B)	E_{MAE}(μeV/V)	E_M(meV/V)
VSi_2N_4	25.00	1.00	1.06	-33.2	282.6
C(N_{in})	24.00	0.96	0.79	-28.9	267.8
C(N_{out})	25.09	1.00	1.04	-13.3	270.6
O(N_{in})	26.00	1.04	1.20	-34.1	259.8
O(N_{out})	26.00	1.04	1.12	-36.2	264.9
MV(N_{in})	26.00	1.04	1.14	-36.2	262.7
MV(N_{out})	26.00	1.04	1.12	-27.8	249.7
MV(Si)	23.11	0.92	0.72	-2.3	233.8
MV(V)	22.02	0.92	0.63	-3.3	203.6