Supplementary Materials

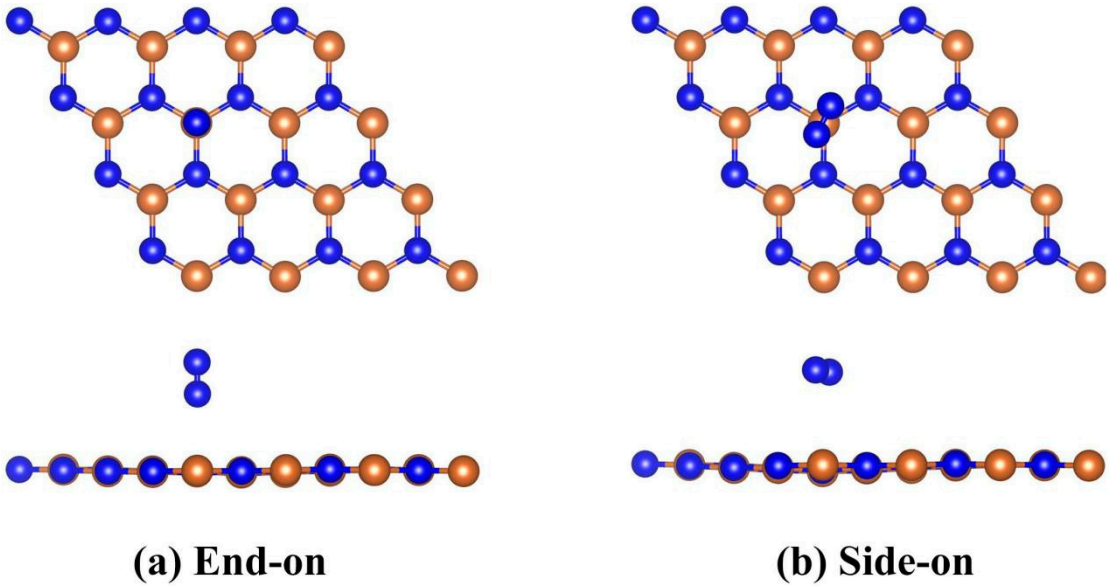


Figure S1. Top and side view of the optimized geometric structures of the adsorption of N_2 on pristine AlN monolayer with the (a) end-on and (b) side-on patterns.

Table S1. Calculated adsorption energies values of N_2 on pristine AlN monolayer with the end-on and side-on patterns .

System	Adsorption energies (eV)	N-N bond lengths (Å)	Al-N distances (Å)
AlN@N_2 end-on	-0.093	1.115	2.727
AlN@N_2 side-on	-0.083	1.115	3.586, 3.537

Table S2.The relative energies (ΔE) of nonmagnetic (NM) and the ferromagnetic (FM) spin polarization, the magnetic moments of FM (M_{tot}) of the different SACs.

	SACs	ΔE (meV)		$M_{tot}(\mu_B)$
		NM	FM	
3d	Sc@AlN	0.0	/	0.0
	Ti@AlN	294.1	0.0	1.0
	V@AlN	1.3	0.0	2.0
	Cr@AlN	0.0	1081.9	3.0
	Mn@AlN	1335.0	0.0	4.0
	Fe@AlN	1523.8	0.0	5.0
	Co@AlN	1069.0	0.0	4.0
	Ni@AlN	573.0	0.0	3.0
	Cu@AlN	391.9	0.0	2.0
	Zn@AlN	90.4	0.0	1.0
4d	Y@AlN	/	/	/
	Zr@AlN	223.4	0.0	1.0
	Nb@AlN	0.0	/	0.0
	Mo@AlN	187.1	0.0	3.0
	Tc@AlN	819.9	0.0	2.0
	Ru@AlN	256.0	0.0	1.0
	Rh@AlN	0.0	/	0.0
	Pd@AlN	157.2	0.0	1.0
	Ag@AlN	254.3	0.0	2.0
	Cd@AlN	113.7	0.0	1.0
5d	Hf@AlN	252.5	0.0	1.0
	Ta@AlN	0.0	/	0.0
	W@AlN	85.6	0.0	0.8
	Re@AlN	940.6	0.0	2.0
	Os@AlN	232.2	0.0	3.0
	Ir@AlN	0.0	/	0.0

	Pt@AlN	129.8	0.0	1.0
	Au@AlN	134.3	0.0	1.0
	Hg@AlN	129.8	0.0	1.0

Table S3. Calculated ΔG_{*H} and ΔG_{*N_2} values of Os@AlN with end-on and side-on adsorption configurations.

System	ΔG_{*H} (eV)	ΔG_{*N_2}(eV)	
		end-on	side-on
Os@AlN	-0.042	-0.074	0.868

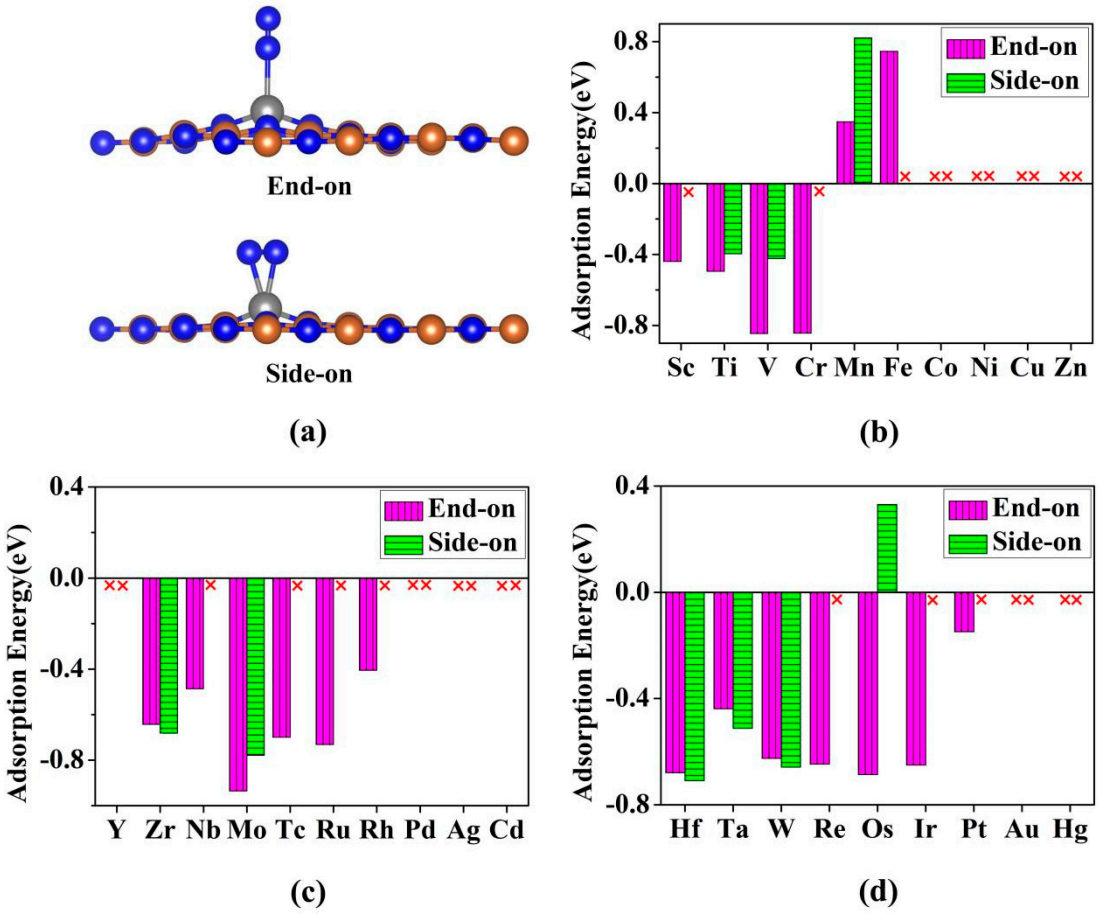


Figure S2. (a) The geometric structures of the adsorption of N_2 on TM@AlN via the end-on and side-on configures. Adsorption energy (E_{ads} in eV) of N_2 adsorbed on (b) 3d TM@AlN, (c) 4d TM@AlN and (d) 5d TM@AlN.

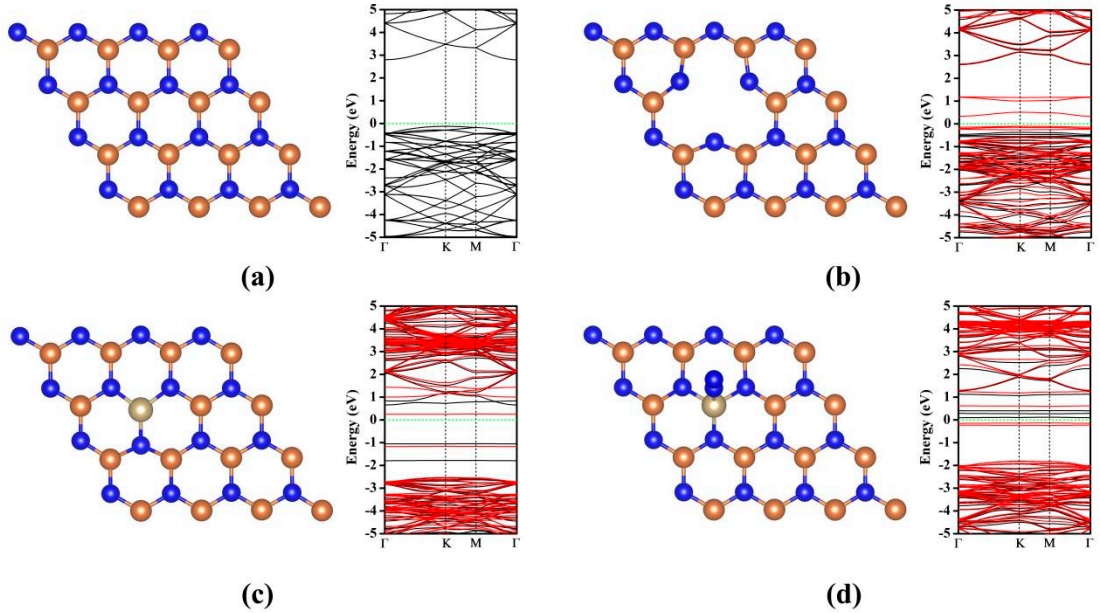


Figure S3. The pristine AlN monolayer (a), defective AlN with Al monovacancy (b), Os@AlN (c) and N_2 adsorption on Os@AlN with end-on configuration (d) of top view and side view, and the corresponding band structures (DFT-PBE level). The black and red dotted lines in the band structures denote the spin-up (↑) and spin-down (↓) channels, respectively. The Fermi-level is set to be zero denoted by green dash line. The orange, blue, and gray denote Al, N, and Os atoms, respectively.

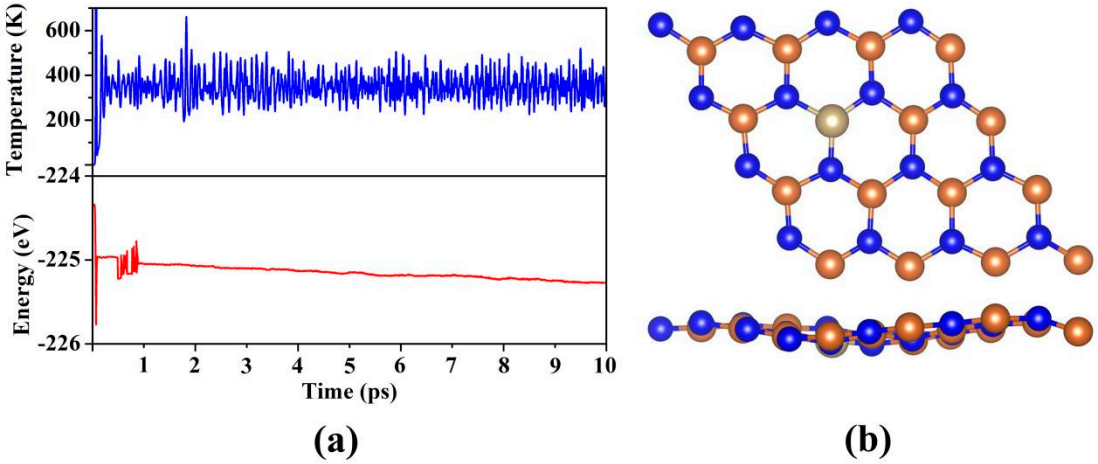


Figure S4. (a) The temperature and energy fluctuations of Os@AlN during 10 ps of AIMD simulation with a time step of 2 fs. (b) The top and side views of Os@AlN after 10 ps of AIMD simulation at T = 350 K.