Supporting Information

Dipole-induced transition from Schottky to Ohmic contact at Janus $MoSiGeN_4$/metal interfaces

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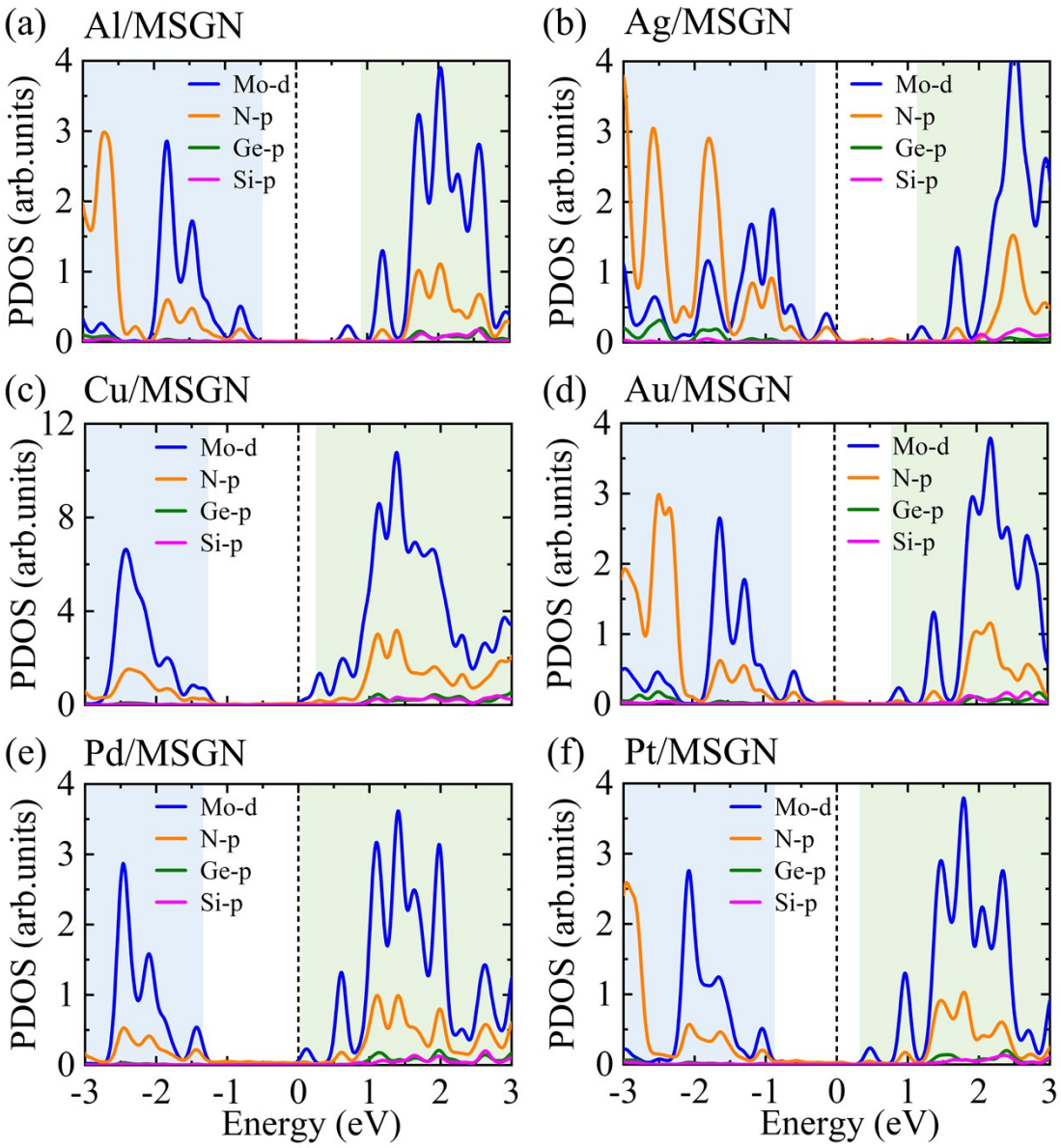

Fig. S1 Partial density of states for (a) Al/MSGN, (b) Ag/MSGN, (c) Cu/MSGN, (d) Au/MSGN, (e) Pd/MSGN, and (f) Pt/MSGN interfaces.

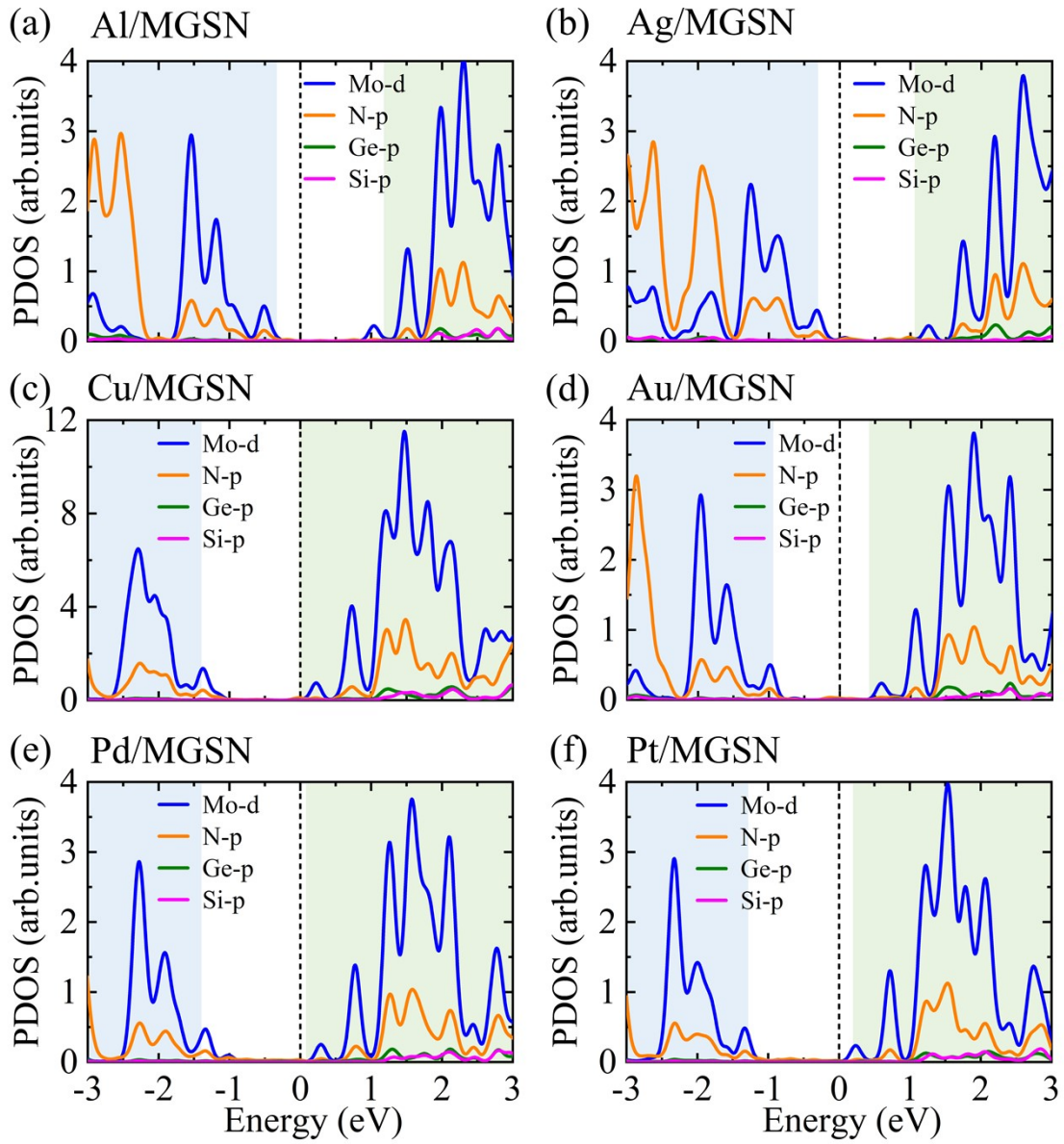

Fig. S2 Partial density of states for (a) Al/MGSN, (b) Ag/MGSN, (c) Cu/MGSN, (d) Au/MGSN, (e) Pd/MGSN, and (f) Pt/MGSN interfaces.

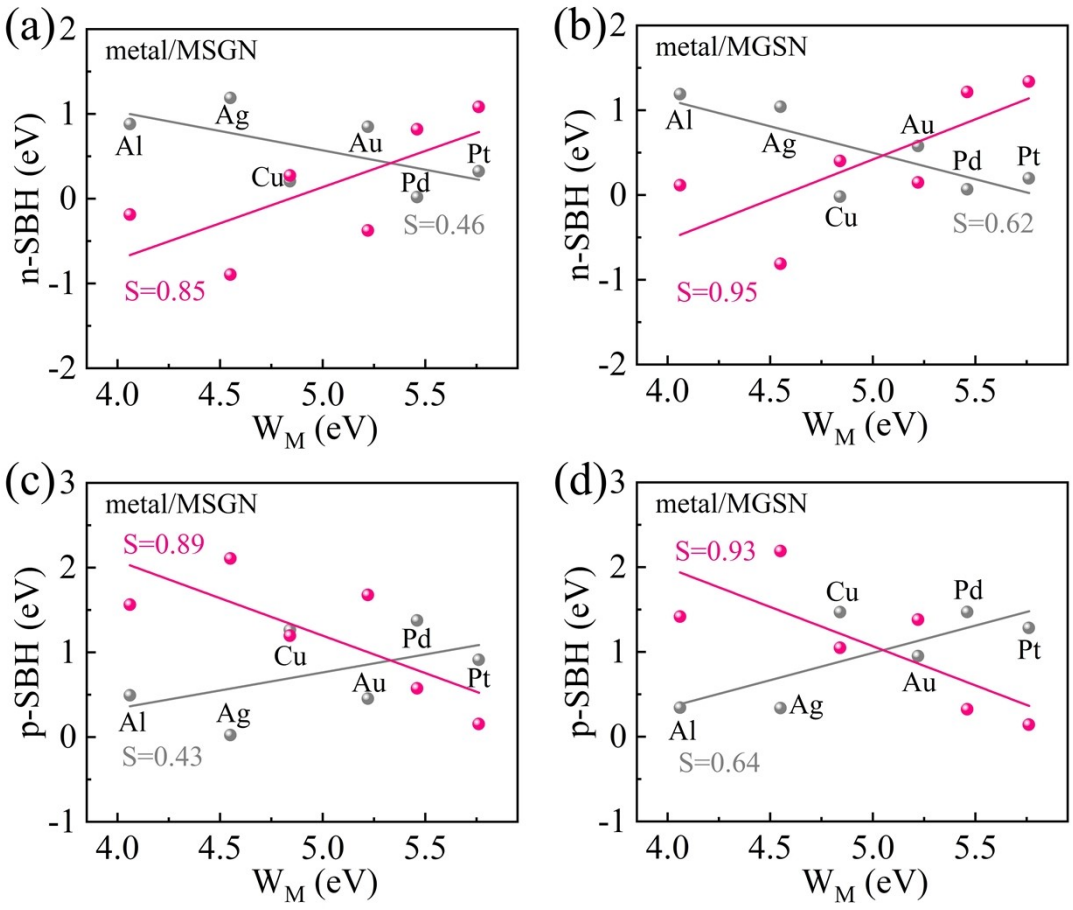

Fig. S3 Schottky-Mott plot for (a, b) n-SBH and (c, d) p-SBH for metal/MSGN and metal/MGSN interfaces. The pink and gray lines represent the pinning factor S with and without ΔV modified, respectively.

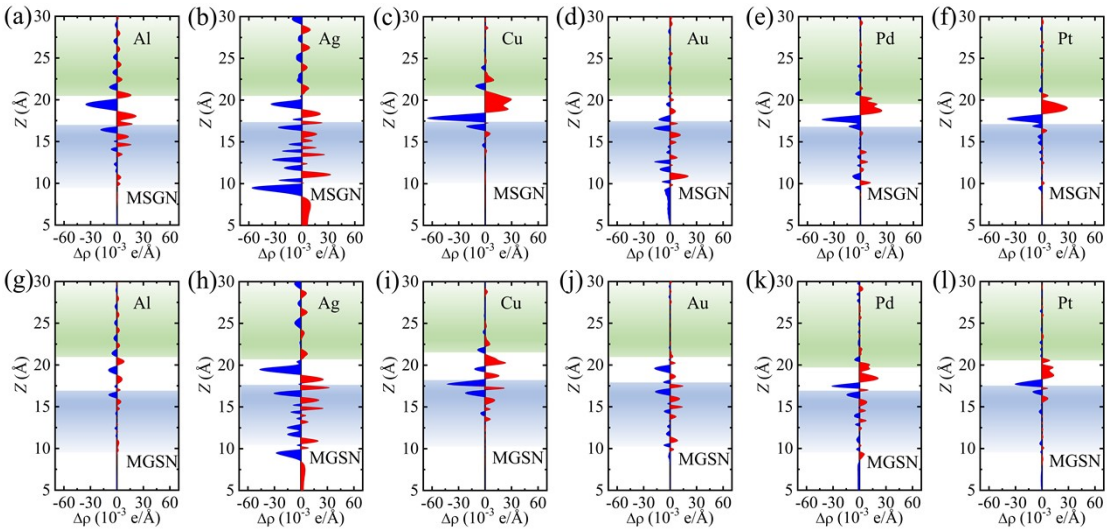

Fig. S4 Plane-averaged differential charge density of (a) Al/MSGN, (b) Ag/MSGN, (c) Cu/MSGN, (d) Au/MSGN, (e) Pd/MSGN, (f) Pt/MSGN, (g) Al/MGSN, (h) Ag/MGSN, (i) Cu/MGSN, (j) Au/MGSN, (k) Pd/MGSN, and (l) Pt/MGSN. The red (blue) color denotes electron accumulation (depletion).

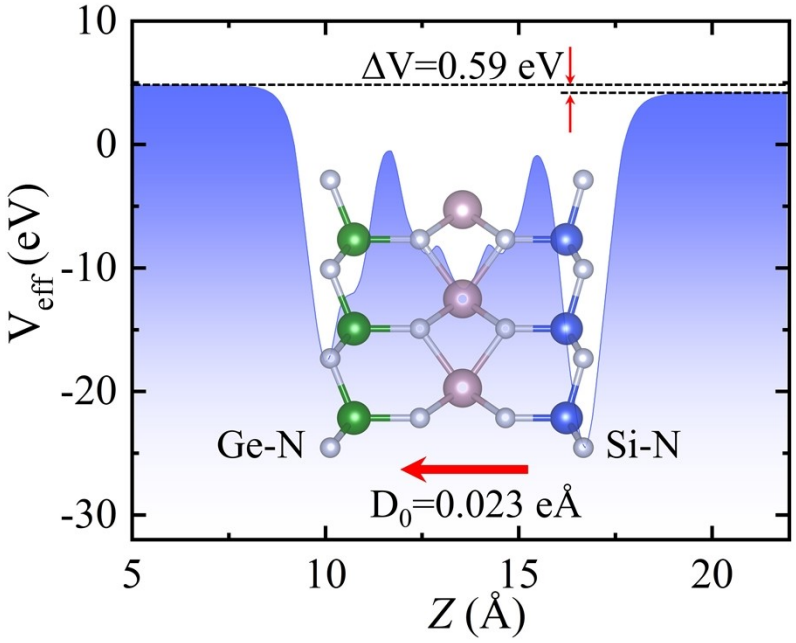

Fig. S5 Calculated plane-averaged electrostatic potentials for $MoSiGeN_4$ monolayer. The values of the intrinsic potential step (ΔV) and dipoles (D_0) for the $MoSiGeN_4$ monolayer are indicated in the figure.

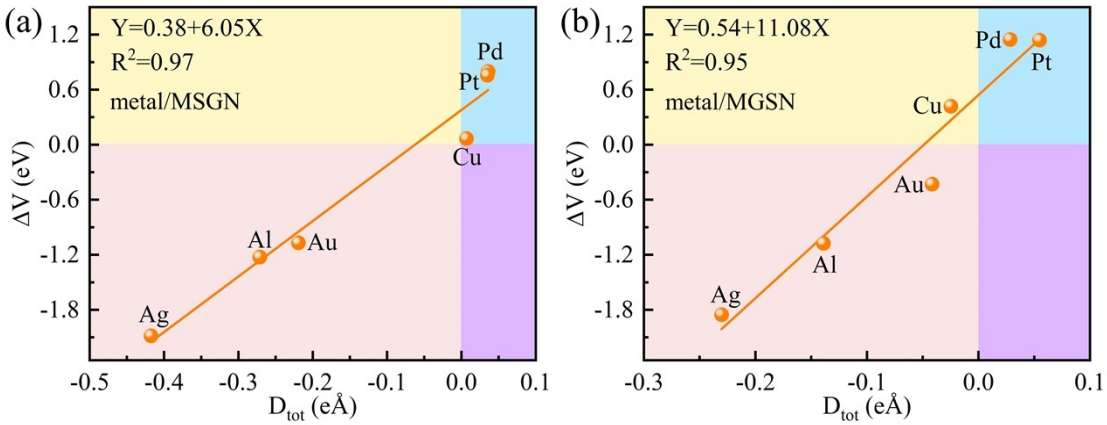

Fig. S6 The change of ΔV with total dipole (D_{tot}) for (a) metal/MSGN and (b) metal/MGSN interfaces.

Table S1 The optimized geometric parameters of Janus $MoSiGeN_4$ monolayer and $MoSi_2N_4$ monolayer, including lattice constants (a, b), bond length of Ge-N (d_1, d_2), Mo-N (d_3, d_4), Si-N (d_5, d_6), and the thickness of the Janus $MoSiGeN_4$ monolayer and $MoSi_2N_4$ monolayer (d_t).

Material	a (Å)	d_1 (Å)	d_2 (Å)	d_3 (Å)	d_4 (Å)	d_5 (Å)	d_6 (Å)	d_t (Å)
$MoSiGeN_4$	2.96	1.841	1.885	2.106	2.108	1.748	1.777	7.261
$MoSi_2N_4$	2.91	1.755	1.747	2.096	2.096	1.747	1.755	7.012

Table S2 The lattice mismatch (δ) between $MoSiGeN_4$ and bulk metals. The work function of 2D metals without strain (W_M) and under strain (W_{M-S}).

metal	Al	Ag	Cu	Au	Pd	Pt
δ (%)	3.53	0.59	1.56	2.63	5.61	5.07
W_M (eV)	4.06	4.55	4.84	5.22	5.46	5.76
W_{M-S} (eV)	4.11	4.46	4.81	5.27	5.24	5.60

Table S3 The minimum ELF value at the center of the line profile curves for metal/$MoSiGeN_4$ interfaces.

ELF	Si-N side	Ge-N side
Al	0.039	0.046
Ag	0.042	0.042
Cu	0.049	0.055
Au	0.039	0.046
Pd	0.058	0.057
Pt	0.052	0.055

Table S4 The values of the n-SBH, p-SBH, W_M, E_f, ΔV, V_0, V_{int}, D_{tot}, D_0, ΔD, d, E_b, and Q for the metal/$MoSiGeN_4$ interfaces.

Systems	n-SBH	p-SBH	W_M	E_f	ΔV	V_0	V_{int}	D_{tot}	D_0	ΔD	d	E_b	Q
Al-MSGN	0.8825	0.4945	4.0600	3.7030	-1.0689	-0.5100	-0.5589	-0.2194	-0.0229	-0.1965	3.4430	-0.2011	0.0297
Ag-MSGN	1.1893	0.0252	4.5500	0.9090	-2.0838	-0.5100	-1.5738	-0.4176	-0.0229	-0.3947	3.0540	-0.6057	0.0599
Cu-MSGN	0.2067	1.2655	4.8360	-0.9260	0.0677	-0.5100	0.5777	0.0068	-0.0229	0.0297	3.1371	-0.3545	0.0095
Au-MSGN	0.8490	0.4549	5.2220	-0.1740	-1.2232	-0.5100	-0.7132	-0.2713	-0.0229	-0.2484	3.1469	-0.4234	0.0154
Pd-MSGN	0.0205	1.3767	5.4600	-1.1730	0.8000	-0.5100	1.3100	0.0359	-0.0229	0.0588	2.6718	-0.3921	-0.0054
Pt-MSGN	0.3252	0.9138	5.7620	-1.6610	0.7583	-0.5100	1.2683	0.0349	-0.0229	0.0578	2.9693	-0.3801	-0.0187
Al-MGSN	1.1908	0.3437	4.0600	2.5130	-1.0747	0.5100	-1.5847	-0.1391	0.0229	-0.1620	3.2618	-0.1697	0.0402
Ag-MGSN	1.0414	0.3392	4.5500	-0.0930	-1.8519	0.5100	-2.3619	-0.2304	0.0229	-0.2533	2.9322	-0.5146	0.0789
Cu-MGSN	-0.0185	1.4703	4.8360	1.0520	0.4205	0.5100	-0.0895	-0.0248	0.0229	-0.0477	3.1402	-0.3468	0.0708
Au-MGSN	0.5788	0.9518	5.2220	1.2990	-0.4297	0.5100	-0.9397	-0.0417	0.0229	-0.0646	2.9896	-0.3506	0.0335
Pd-MGSN	0.0689	1.4714	5.4600	1.2290	1.1463	0.5100	0.6363	0.0284	0.0229	0.0054	2.6675	-0.3840	0.0309
Pt-MGSN	0.1976	1.2846	5.7620	1.8490	1.1412	0.5100	0.6312	0.0547	0.0229	0.0318	2.8791	-0.3734	0.0045

Table S5 The tunnel barriers height (Φ_{TB}), tunnel barrier width (D_{TB}), tunneling probability (TP), and the tunneling specific resistivity (ρ_t) for metal/MGSN (Ge-N) and metal/MSGN (Si-N) interfaces.

	Φ_{TB} (eV)		D_{TB} (Å)		TP (%)		ρ_t (10^{-9} Ω·cm^2)	
	Si-N	Ge-N	Si-N	Ge-N	Si-N	Ge-N	Si-N	Ge-N
Al	3.13	3.34	1.69	1.61	14.20	14.64	1.865	1.689
Ag	3.35	3.60	1.43	1.28	18.11	20.49	1.421	1.310
Cu	3.47	3.87	1.46	1.56	16.96	13.50	1.427	1.600
Au	4.41	3.85	1.61	1.34	11.01	17.99	1.834	1.242
Pd	2.79	3.50	0.92	0.95	36.68	31.32	0.056	0.066
Pt	3.78	2.62	1.28	0.94	19.68	37.01	1.236	0.058