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Supporting Information

Achieving real Ohmic contact by the dual protection of outer layer atoms and surface functionalization in 2D metal Mxenes/$MoSi_2N_4$ heterostructures

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Table S1. W_M represents the work function of 2D metal Mxenes. ΔV represents the potential step. △Q represents the number of charges transferred by Mxenes after contact, where "-" represents the loss of charge of Mxenes. ω_{TB} and Φ_{TB} respectively represent the width and height of tunneling barrier, Φ_{Bp} and Φ_{Bn} are the SBH of hole and electron, where OC represents the ohmic contact.

	W_M	ΔV	△Q(|e|)	ω_{TB}	Φ_{TB}	Φ_{Bp}	Φ_{Bn}
Ti_4C_3	4.067	-0.58	-0.161	0.245	0.124	1.393	OC(-0.396)
$Ti_4C_3F_2$	4.742	-0.001	-0.008	2.037	4.057	0.473	0.639
$Ti_4C_3O_2$	6.087	0.523	0.032	1.967	5.002	OC(-0.17)	1.791
$Ti_4C_3O_2H_2$	1.893	-1.01	-0.158	0.603	0.684	1.483	OC(-0.446)
V_4C_3	4.55	-0.672	-0.146	0.182	0.106	1.779	OC(-0.151)
$V_4C_3F_2$	5.782	-0.019	0.017	2.044	5.015	0.1	1.445
$V_4C_3O_2$	6.624	-0.95	0.035	2.023	5.573	OC(-0.085)	1.657
$V_4C_3O_2H_2$	1.787	1.315	-0.144	0.68	0.637	1.913	OC(-0.375)
Zr_4C_3	4.408	-0.768	-0.631	0	0	2.366	OC(-0.813)
$Zr_4C_3F_2$	3.573	0.164	-0.164	1.626	2.866	1.879	OC(-0.164)
$Zr_4C_3O_2$	5.35	-0.007	0.008	1.847	4.511	0.098	1.753
$Zr_4C_3O_2H_2$	2.158	0.986	-0.533	0.749	0.716	2.281	OC(-0.561)
Nb_4C_3	4.348	-1.016	-0.456	0	0	2.418	OC(-0.109)
$Nb_4C_3F_2$	4.989	0.013	-0.013	1.733	3.901	0.97	1.217
$Nb_4C_3O_2$	5.757	-0.015	0.026	1.768	4.723	0.075	2.217
$Nb_4C_3O_2H_2$	1.818	1.15	-0.366	0.856	0.902	2.489	OC(-0.065)
Hf_4C_3	4.526	-0.742	-0.705	0	0	2.711	OC(-0.915)
$Hf_4C_3F_2$	3.079	0.249	-0.167	1.283	2.304	1.921	OC(-0.118)
$Hf_4C_3O_2$	5.39	-0.074	0.036	1.493	3.981	0.543	1.5
$Hf_4C_3O_2H_2$	2.5	1.101	-0.591	0.487	0.419	2.174	OC(-0.284)

Fig. S1 The projected band structure, projected density of states(The red dots represent $MoSi_2N_4$ and the grey dots represent Mxenes), 2D/3D charge density difference and effective potential of the 2D metal Mxenes/$MoSi_2N_4$ heterostructures.