Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information:

Tuning Schottky barriers for monolayer GaSe FETs by exploiting weak Fermi level pinning effect

Nanshu Liu, Si Zhou*, Nan Gao, Jijun Zhao

Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education, Dalian 116024, China

* Corresponding authors. Email: sizhou@dlut.edu.cn

Table S1 Interlayer distance (*d*) and Schottky barrier in the vertical direction for electron carrier (Φ^e_V) calculated by using PBE-D3 and vdW-optB86 functionals.

		V_2C	Au	Nb_2CO_2
PBE-D3	*d* (Å)	2.25	2.63	2.81
	Φ^e_V (eV)	0	0.31	1.70
vdW-optB86	*d* (Å)	1.97	2.90	2.96
	Φ^e_V (eV)	0	0.13	1.72

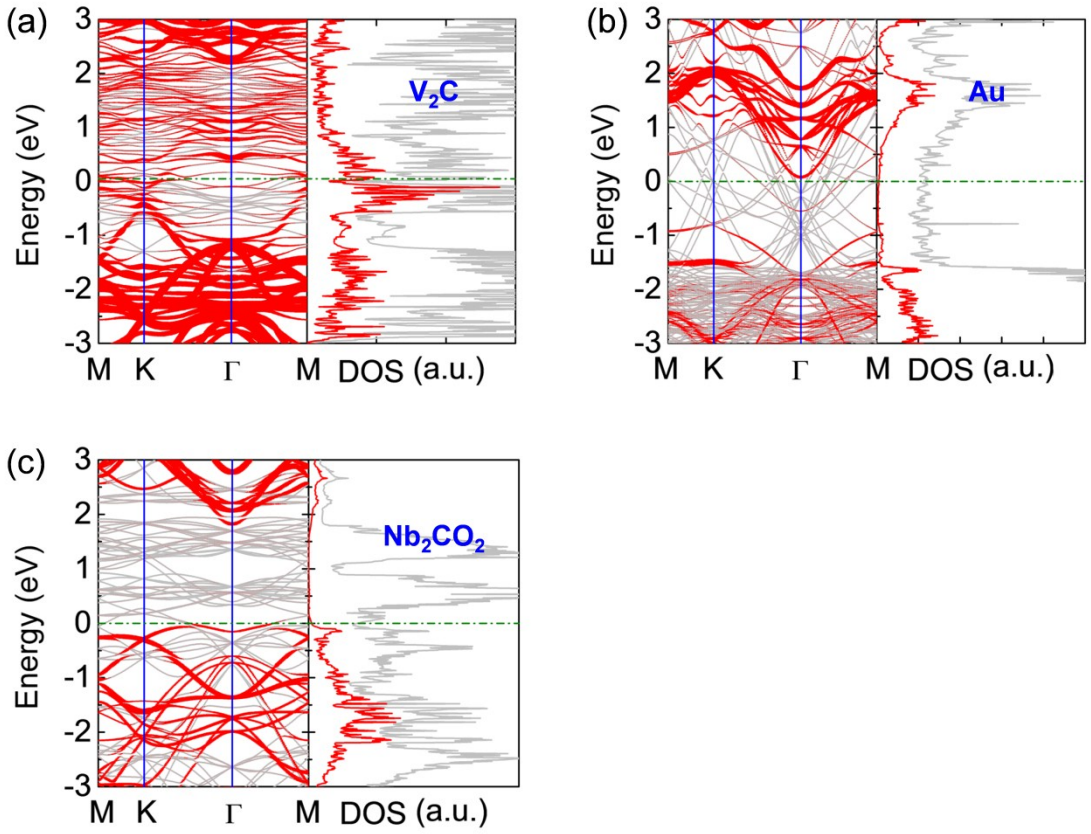

Fig. S1 Electronic band structures (left panels) and density of states (DOS) (right panels) calculated by using the vdW-optB86b functional for GaSe monolayer in contact with (a) bare MXene V_2C, (b) Au(111) surface, and (c) O-terminated MXene Nb_2CO_2, respectively. The red lines show the bands or DOS from the GaSe sheet, and the line width is proportional to the weight. The grey lines show the bands or DOS from the electrode materials. The Fermi level is set to zero.

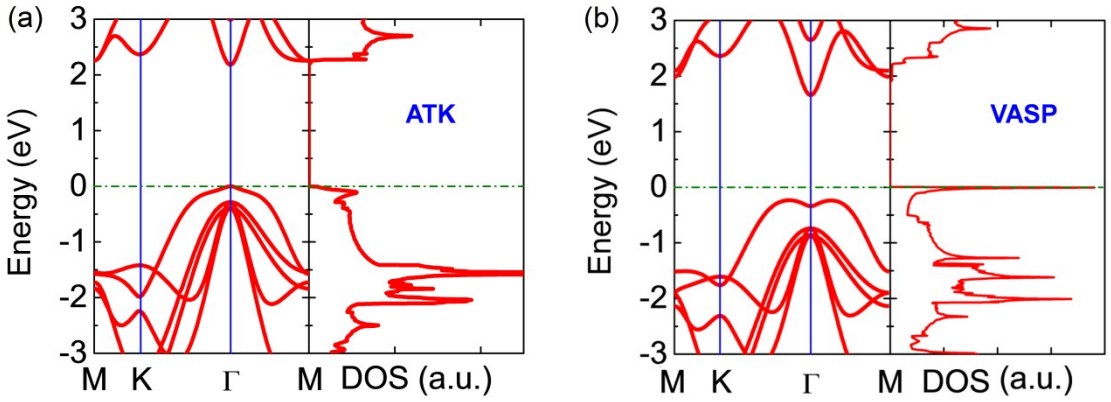

Fig. S2 Electronic band structures (left panels) and density of states (DOS) (right panels) of GaSe monolayer calculated by (a) ATK and (b) VASP. The Fermi level is set to zero.

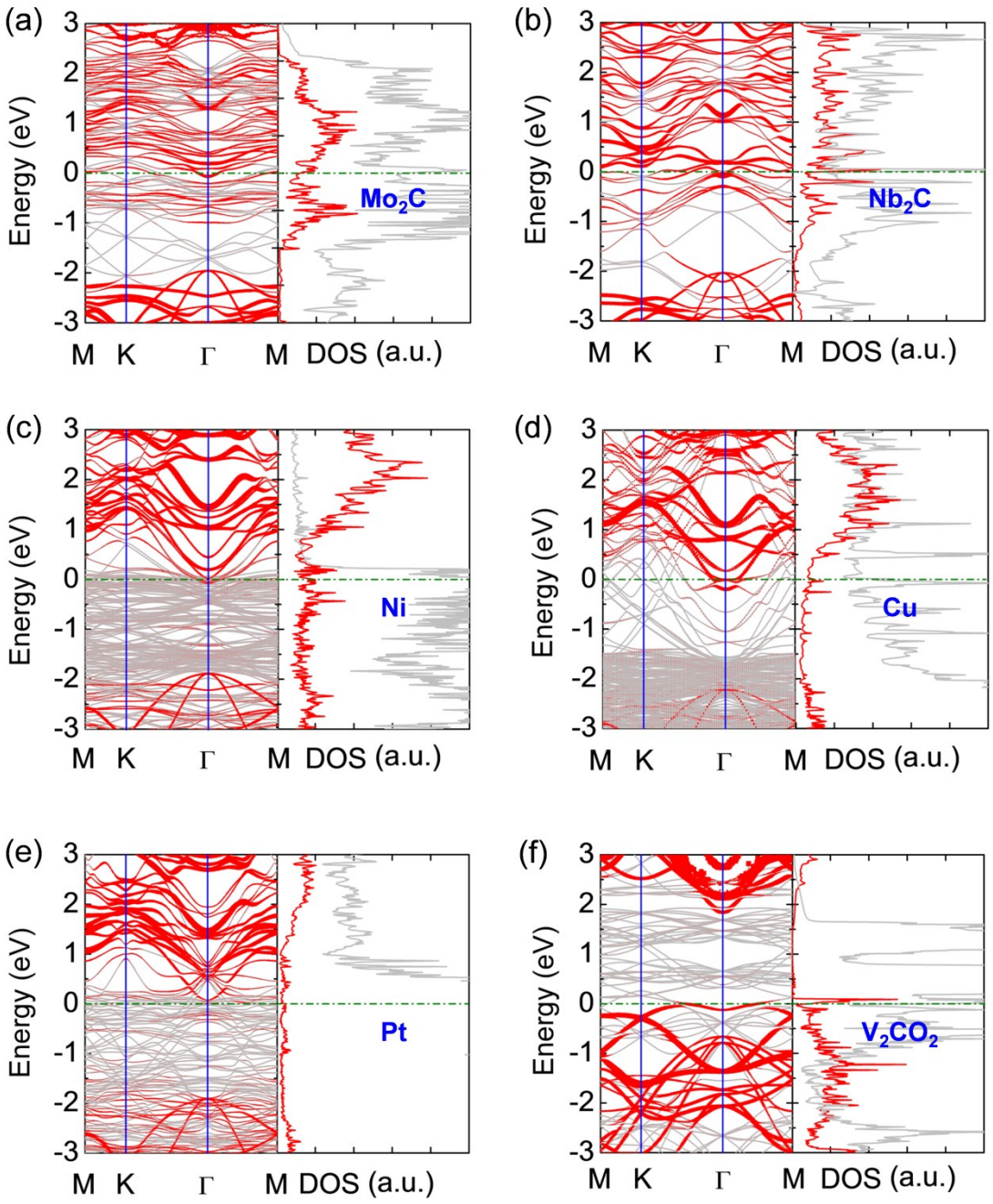

Fig. S3 Electronic band structures (left panels) and density of states (DOS) (right panels) in contact with (a)Mo_2C, (b)Nb_2C, (c)Ni, (d) Cu, (e) Pt, and (f) V_2CO_2, respectively. The red lines show the bands or DOS from the GaSe sheet, and the line width is proportional to the weight. The grey lines show the bands or DOS from the electrode materials. The Fermi level is set to zero.

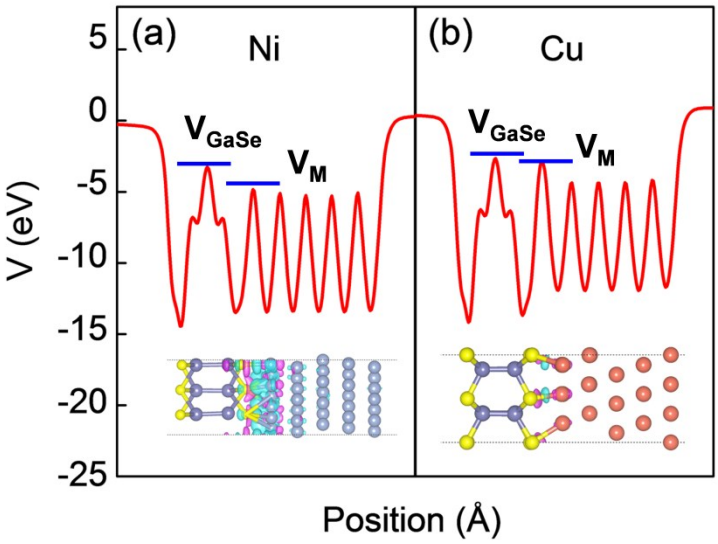

Fig. S4 Electrostatic potential profiles along vertical direction for (a) GaSe/Ni and (b)GaSe/Cu junctions. The insets show the corresponding interfacial structures and differential charge densities. The cyan and magenta colors represent the charge accumulation and depletion regions with an isosurface value of 0.003 e/Å^3, respectively.

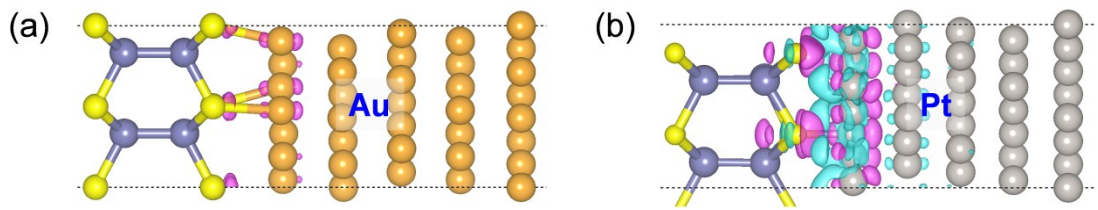

Fig. S5 Interfacial structures and differential charge densities for (a) GaSe/Au and (b) GaSe/Pt junctions. The cyan and magenta colors represent the charge accumulation and depletion regions with an isosurface value of 0.003 e/Å^3, respectively.