Electronic supplementary information

Promising electron mobility and high thermal conductivity in Sc_2CT_2 (T=F, OH) MXenes

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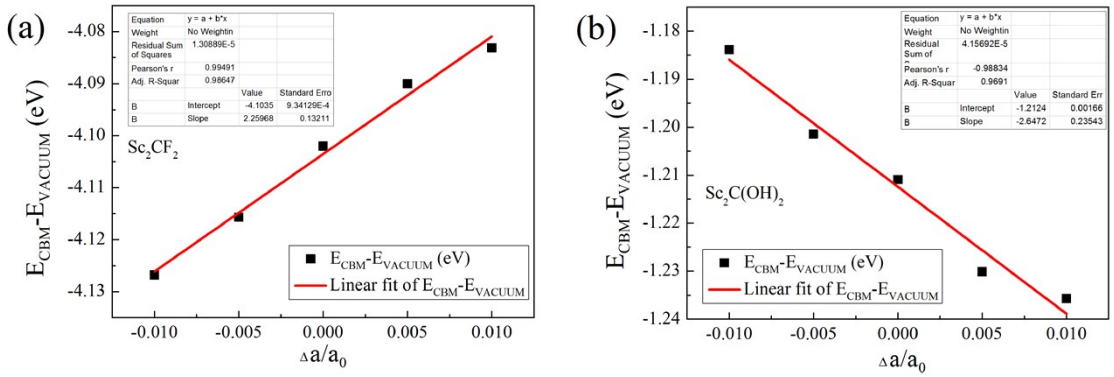

Figure S1 (a) Linear fitting function of the Sc_2CF_2 CBM under uniaxial strains along zigzag direction. (b) Linear fitting function of the $Sc_2C(OH)_2$CBM under uniaxial strains along zigzag direction.

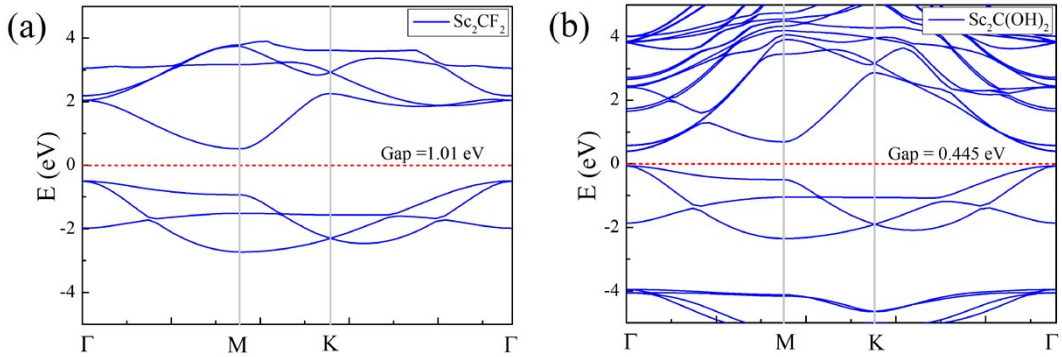

Figure S2 (a) the electronic energy band of the Sc_2CF_2 MXene; (b) the electronic energy band of the $Sc_2C(OH)_2$ MXene based on their primitive cells[1].

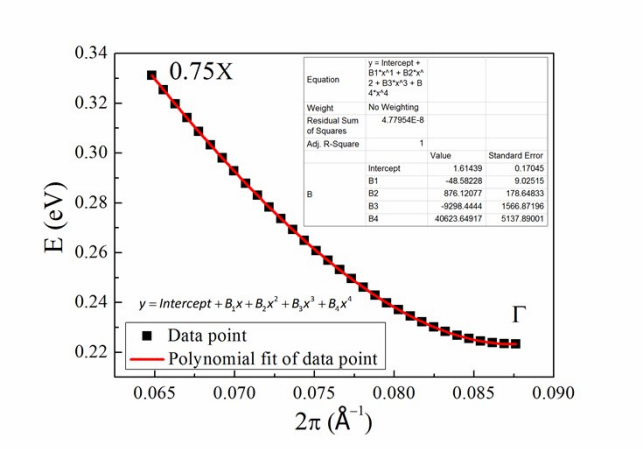

Figure S3 the polynomial fitting function of the electronic energy band near Γ point for calculating the electron effective mass along the Sc_2CF_2 zigzag direction.

In order to estimate the carrier's effective mass, the polynomial function to the fourth order is adopted to fit the relationship between the energy data points and the wave vectors along the transport direction. As an example, we discuss the determination of the electron effective mass along the Sc_2CF_2's zigzag direction in detail. Thirty energy data points [one fourth of the total data points along the zigzag (x-) direction] near the CBM are adopted (the Γ point is included) to fit the polynomial function: $y = Intercept + B_1x + B_2x^2 + B_3x^3 + B_4x^4$. With the fitting function, the second derivative value at Γ point is indeed calculated as: $\frac{\partial^2 y}{\partial x^2}|_{x=\Gamma} = 2B_2 + 6B_3x + 12B_4x^2|_{x=\Gamma}$. According to the definition of carrier effective mass $m^* = |\hbar^2(\frac{\partial^2 y}{\partial x^2})^{-1}|$, the electron effective mass along the Sc_2CF_2 zigzag direction is calculated. Similarly, the electron effective mass along armchair direction, and the hole effective masses in both directions are determined.

Table S1 the electron mobilities of the Sc_2CT_2 (T=F, OH) MXenes under compressed and stretched uniaxial strains.

System	Direction	Strain (%)	m_x^*/m_0	m_y^*/m_0	μ_x ($10^3 cm^2V^{-1}s^{-1}$)	μ_y ($10^3 cm^2V^{-1}s^{-1}$)
Sc_2CF_2	Zigzag	-0.5	0.244	1.49	5.26	1.06
	(x-)	0.5	0.264	1.55	4.57	0.955
	Armchair	-0.5	0.252	1.68	4.70	0.867
	(y-)	0.5	0.255	1.60	4.75	0.926
$Sc_2C(OH)_2$	Zigzag	-0.5	0.518	0.501	2.02	1.98
	(x-)	0.5	0.527	0.507	1.97	1.93
	Armchair	-0.5	0.526	0.498	1.98	1.98
	(y-)	0.5	0.522	0.533	1.94	1.79

1. X.-H. Zha, K. Luo, Q. Li, Q. Huang, J. He, X. Wen and S. Du, *EPL (Europhysics Letters)*, 2015, **111**, 26007.