Can magneto-transport properties provide insight into the functional groups in semiconducting MXenes?

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Figure S1: Side view of Sc\(_2\)CF\(_2\) (a) I, (b) II, (c) III and (d) IV configurations. Side and top view of optimized structure of Sc\(_2\)C functionalized by (e,h) F, (f,i) O and (g,j) OH. Lavender, brown, blue, red and white balls correspond to Sc, C, F, O and H atoms respectively.
Figure S2: For Sc$_2$CF$_2$, the conduction band edge shift position for uniaxial strain along (a) x, (c) y, and (e) z directions. The relationship between total energy and strain along (b) x, (d) y, and (f) z directions are given for Sc$_2$CF$_2$. 
Table S1: Deformation potential calculation for Sc$_2$CF$_2$: $E(\epsilon) = a\epsilon + b$, $D_A = \frac{\partial E}{\partial \epsilon} = a$

| Parameter | LA  | TA  | ZA  |
|-----------|-----|-----|-----|
| a         | -2.166 | -2.17 | -6.842 |
| Standard error | ±0.07429 | ±0.07243 | ±0.0006 |
| b         | -1.541 | -1.541 | -1.539 |
| Standard error | ±0.00053 | ±0.00051 | ±0.0004 |

Table S2: Elastic moduli calculation for Sc$_2$CF$_2$: $E(\epsilon) = a\epsilon^2 + b\epsilon + c$, $C = \frac{\partial^2 E}{\partial \epsilon^2} = 2a$

| Parameter | LA  | TA  | ZA  |
|-----------|-----|-----|-----|
| a         | 69.218 | 69.205 | 49.620 |
| Standard error | ±0.522 | ±0.517 | ±0.142 |
| b         | -0.124 | -0.124 | -0.014 |
| Standard error | ±0.0031 | ±0.0031 | ±0.0008 |
| c         | -38.451 | -38.451 | -38.451 |
| Standard error | ±0.00003 | ±0.00003 | ±0.000009 |

Figure S3: Scattering rates versus energy due to acoustic phonons: (a) Sc$_2$CF$_2$, (b) Sc$_2$CO$_2$ and (c) Sc$_2$C(OH)$_2$. 
Figure S4: Conductivity as a function of temperature: (a) Sc$_2$CF$_2$, (b) Sc$_2$CO$_2$ and (c) Sc$_2$C(OH)$_2$.

Figure S5: For a given concentration ($n=5\times10^{12}$ cm$^{-2}$), the difference in Hall scattering factor $\Delta r$ calculated using RTA and Rode approach as a function of temperature.
Figure S6: The Hall scattering factor as a function of concentration at different temperatures (a)Sc$_2$CF$_2$, (b)Sc$_2$CO$_2$ and (c)Sc$_2$C(OH)$_2$. (d) Hall factor of Sc$_2$CF$_2$, Sc$_2$CO$_2$ and Sc$_2$C(OH)$_2$ at 300 K.
Table S3: At Fermi energy ($E_F$) for doping concentration of $4 \times 10^{13}$ cm$^{-2}$ and temperature of 300 K

| Material  | $g(E)$   | $h(E)$   | $\frac{h(E)}{((g(E))^2}$ |
|-----------|----------|----------|-----------------------------|
| $\text{Sc}_2\text{CF}_2$ | $1.63 \times 10^{-7}$ | $-5.97 \times 10^{-12}$ | -224.69                     |
| $\text{Sc}_2\text{CO}_2$ | $4.52 \times 10^{-7}$ | $-3.60 \times 10^{-11}$ | -176.21                     |
| $\text{Sc}_2\text{C(OH)}_2$ | $6.80 \times 10^{-7}$ | $-8.96 \times 10^{-11}$ | -193.77                     |