Electronic Supplementary Information

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

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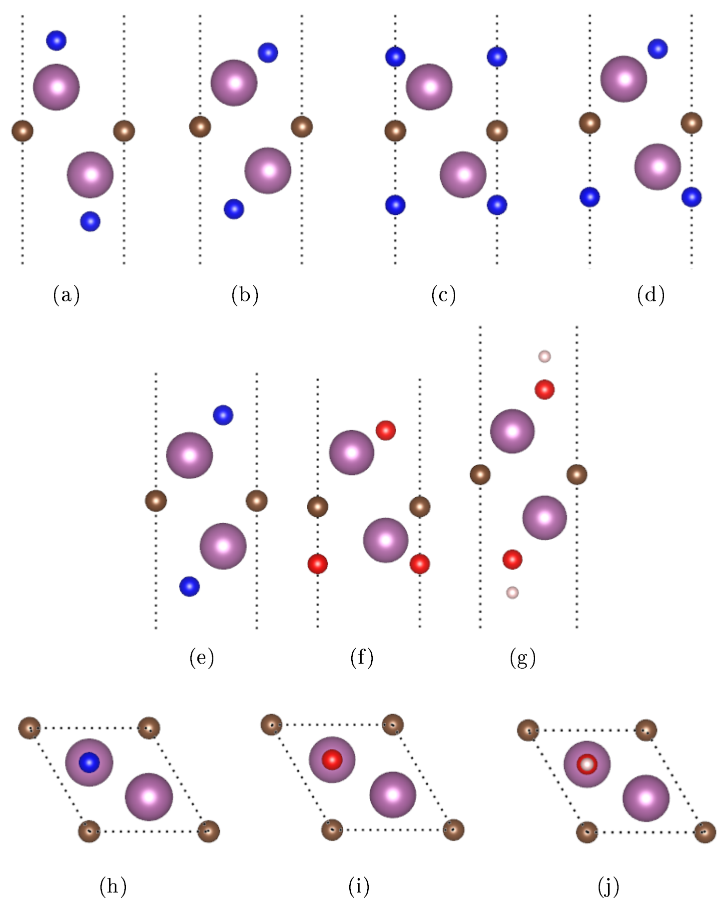
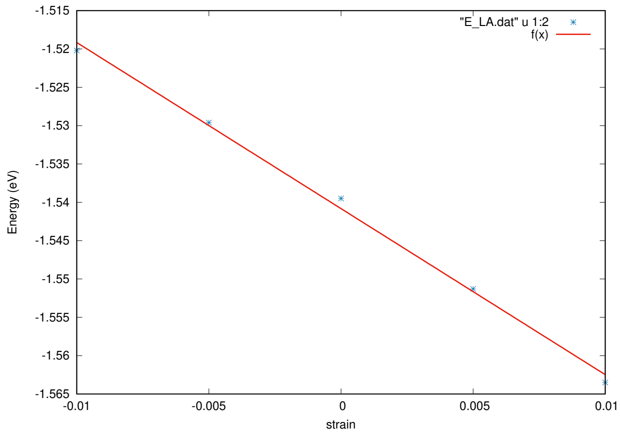
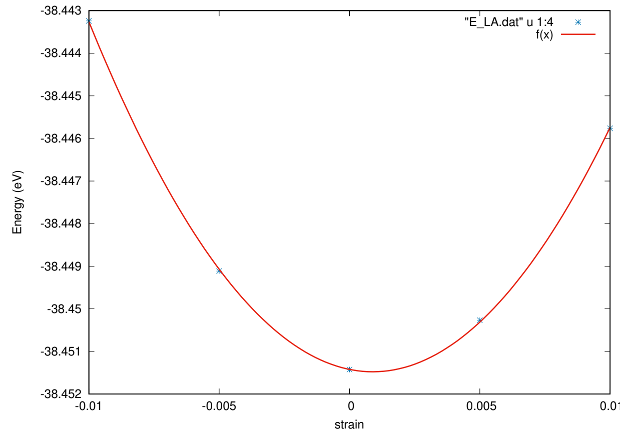


Figure S1: Side view of Sc_2CF_2 (a) I, (b) II, (c) III and (d) IV configurations. Side and top view of optimized structure of Sc_2C functionalized by (e,h) F, (f,i) O and (g,j) OH. Lavendar, brown, blue, red and white balls correspond to Sc, C, F, O and H atoms respectively.



(a)



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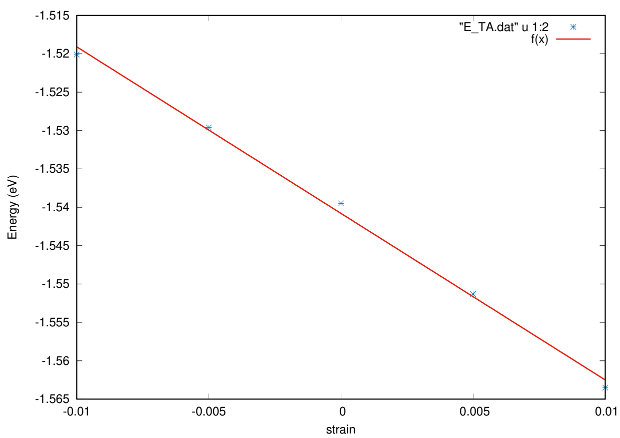

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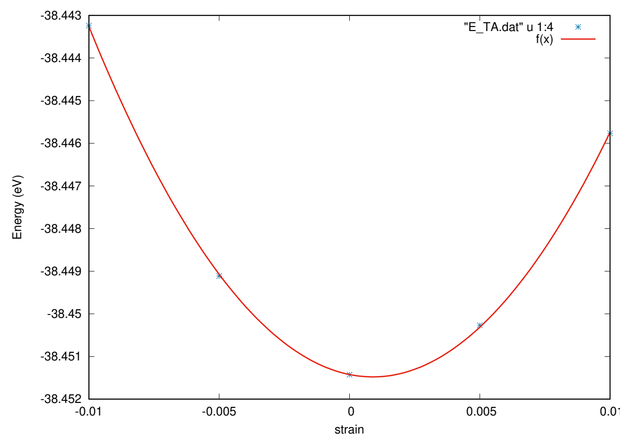

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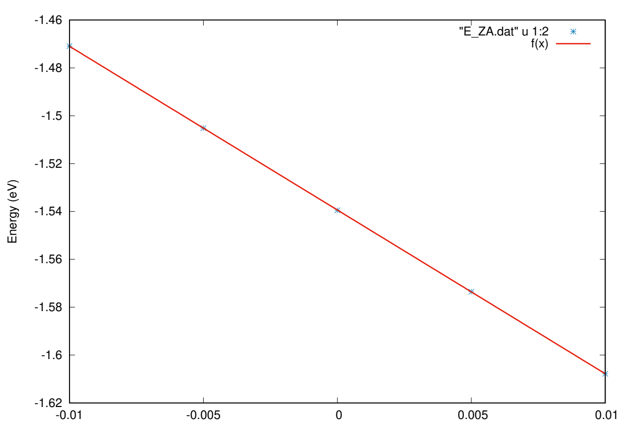

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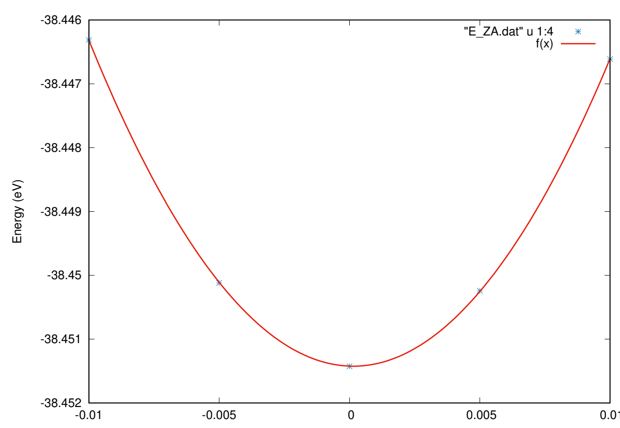


(f)

Figure S2: For Sc_2CF_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_2CF_2.

Table S1: Deformation potential calculation for Sc_2CF_2: $E(\epsilon)$=aϵ+b, $D_A=\frac{\partial E}{\partial \epsilon}$=a

	LA	TA	ZA
Parameter a	-2.166	-2.17	-6.842
Standard error	±0.07429	±0.07243	±0.0006
Parameter b	-1.541	-1.541	-1.539
Standard error	±0.00053	±0.00051	±0.00004

Table S2: Elastic moduli calculation for Sc_2CF_2: $E(\epsilon)$=aϵ^2+bϵ+c, $C=\frac{\partial^2 E}{\partial \epsilon^2}$=2a

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

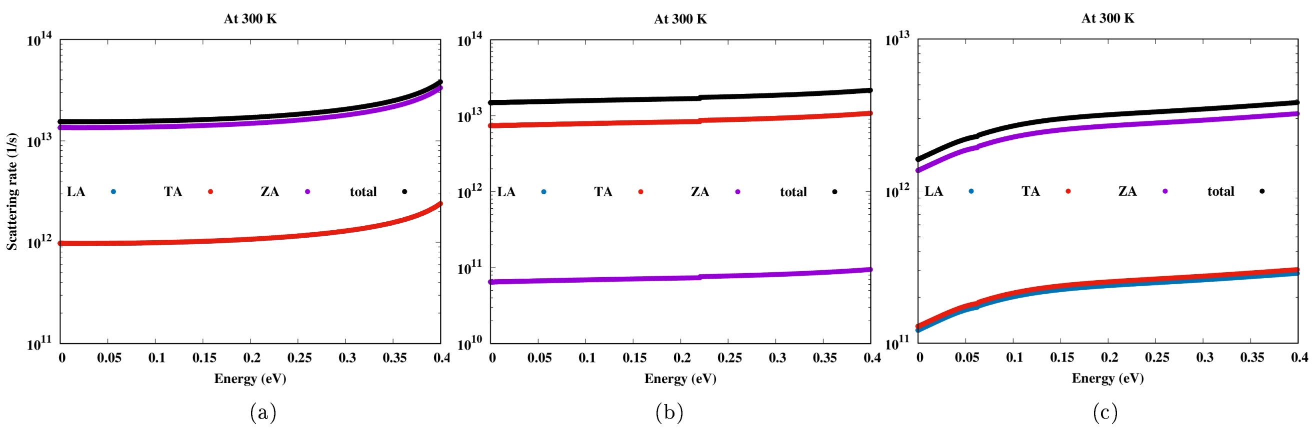
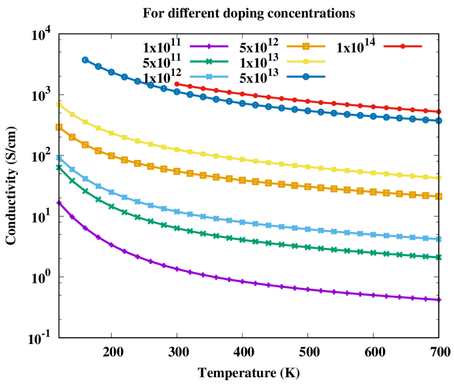
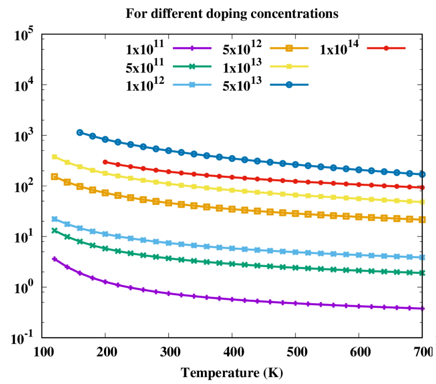


Figure S3: Scattering rates versus energy due to acoustic phonons: (a) Sc_2CF_2, (b) Sc_2CO_2 and (c) $Sc_2C(OH)_2$.



(a)



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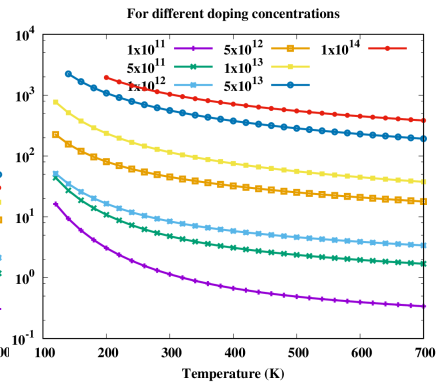
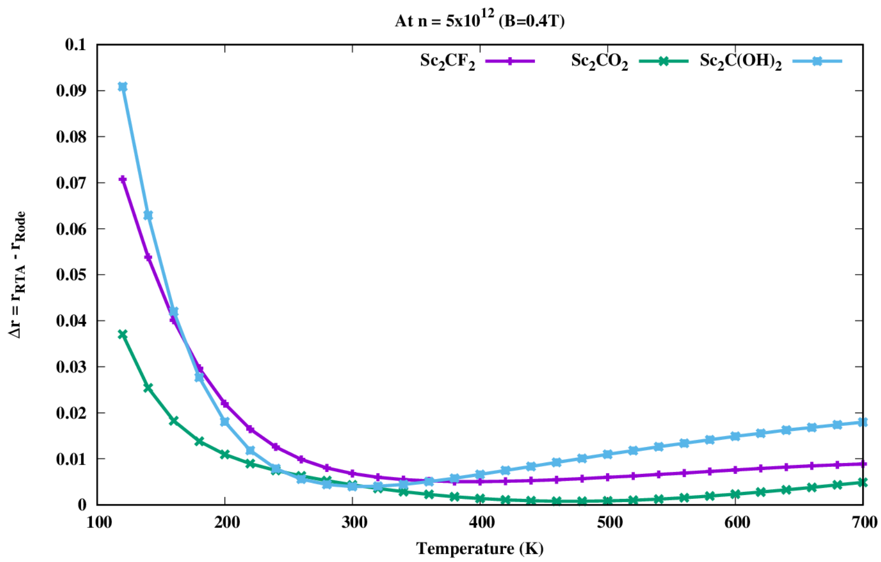


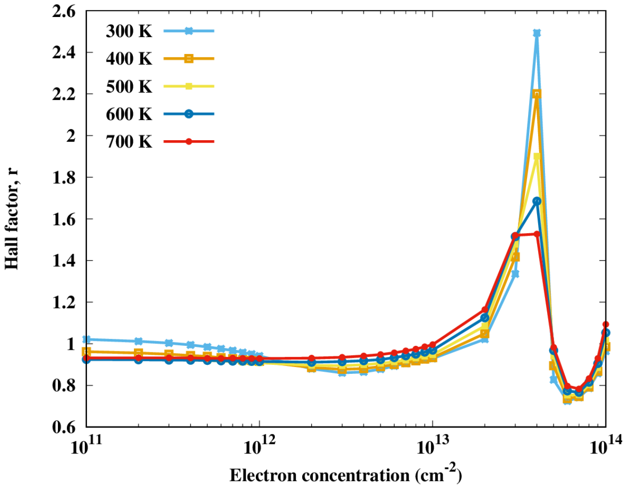
(c)

Figure S4: Conductivity as a function of temperature: (a) Sc_2CF_2, (b) Sc_2CO_2 and (c) $Sc_2C(OH)_2$.

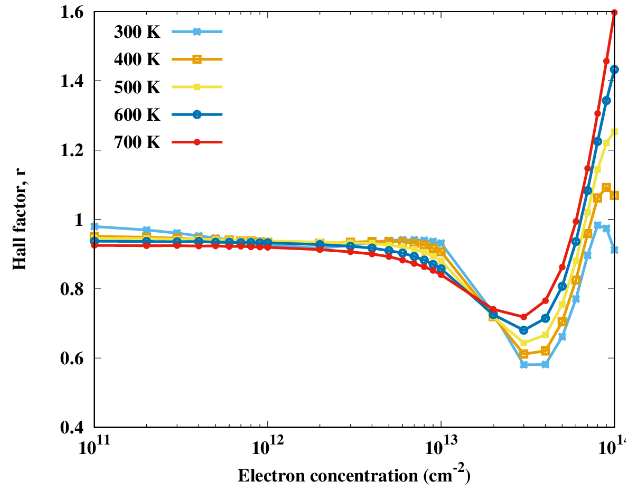


(a)

Figure S5: For a given concentration ($n=5\times10^{12}$ cm^{-2}), the difference in Hall scattering factor Δr calculated using RTA and Rode approach as a function of temperature.



(a)



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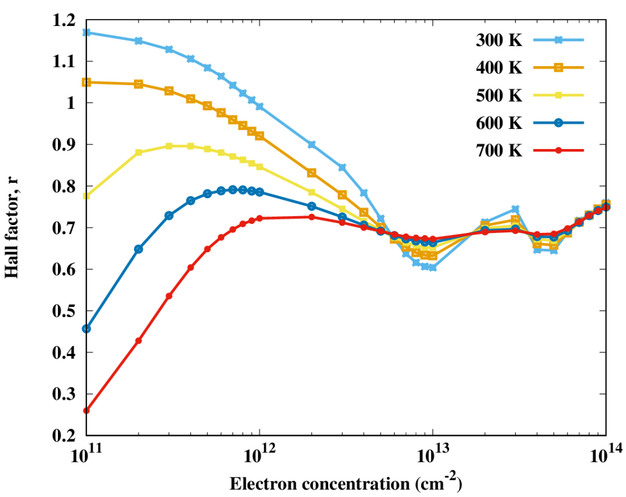
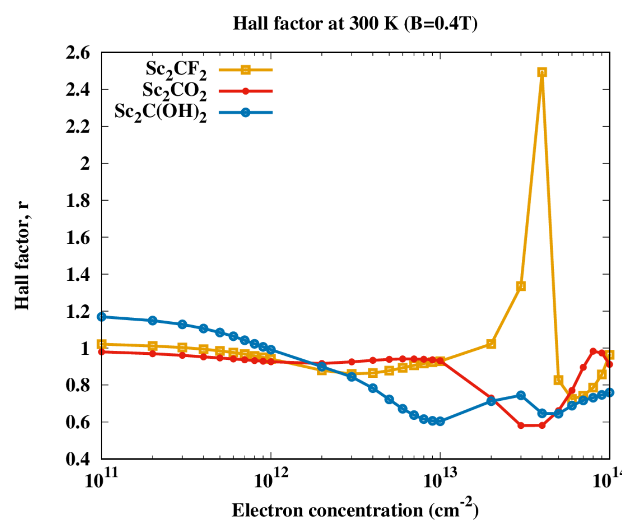


(c)



(d)

Figure S6: The Hall scattering factor as a function of concentration at different temperatures (a)Sc_2CF_2, (b)Sc_2CO_2 and (c)$Sc_2C(OH)_2$. (d) Hall factor of Sc_2CF_2, Sc_2CO_2 and $Sc_2C(OH)_2$ at 300 K.

Table S3: At Fermi energy (E_F) for doping concentration of 4×10^{13} cm^{-2} and temperature of 300 K

Material	g(E)	h(E)	$\frac{h(E)}{((g(E))^2}$
Sc_2CF_2	1.63×10^{-7}	-5.97×10^{-12}	-224.69
Sc_2CO_2	4.52×10^{-7}	-3.60×10^{-11}	-176.21
$Sc_2C(OH)_2$	6.80×10^{-7}	-8.96×10^{-11}	-193.77