Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supplemental material

to

Investigation of Van der Waals interactions in two-dimensional MXenes via first-principles simulations

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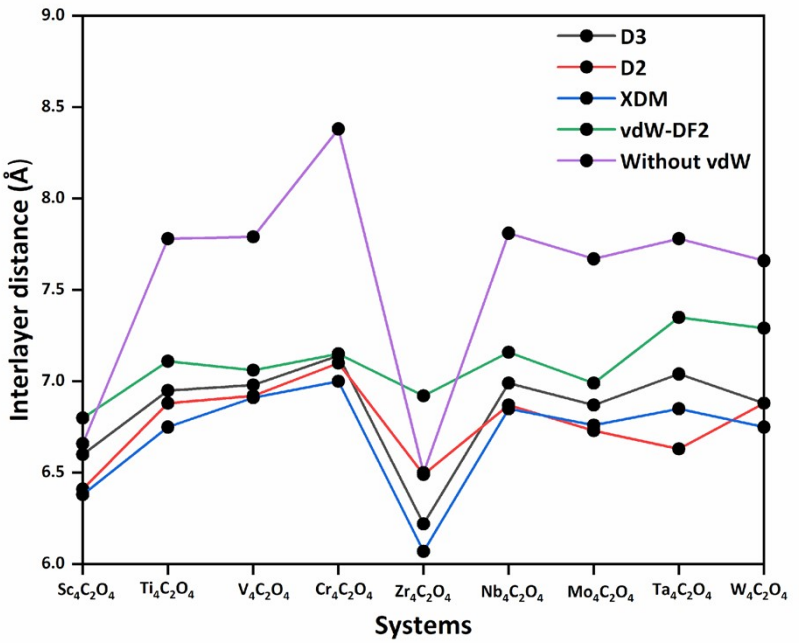

Figure S1 Interlayer distance values of 9 different oxygen terminated MXenes calculated with 4 different dispersion correction and without correction

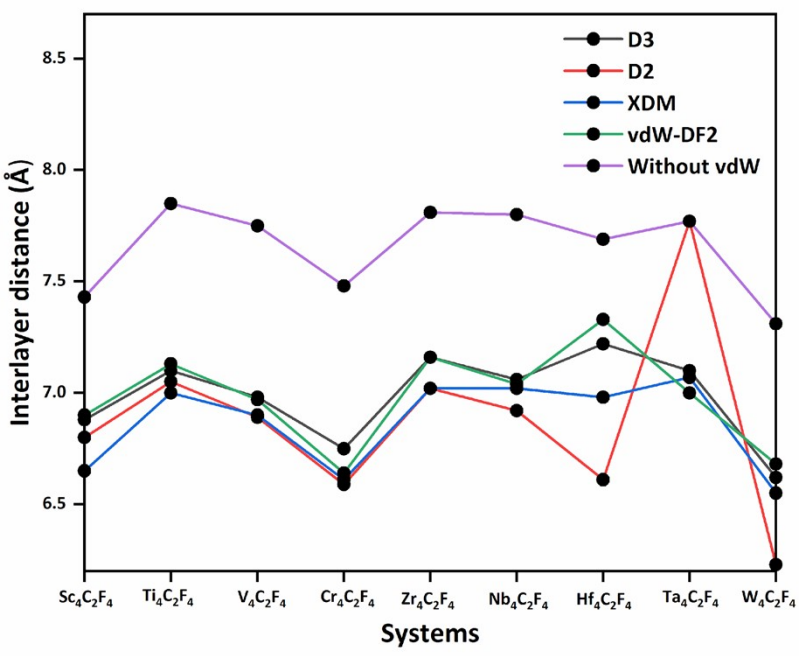

Figure S2 Interlayer distance values of 9 different fluorine terminated MXenes calculated with 4 different dispersion correction and without correction

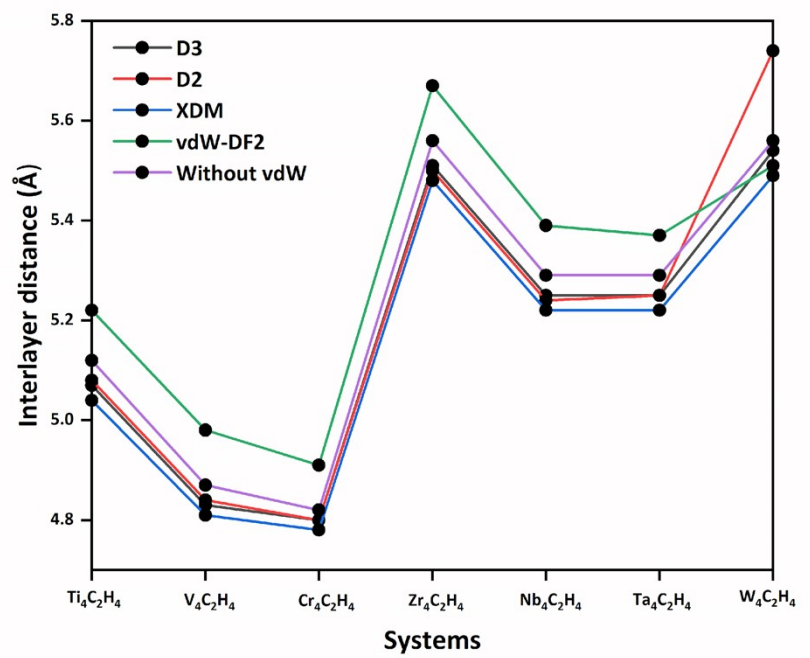

Figure S3 Interlayer distance values of 7 different hydrogen terminated MXenes calculated with 4 different dispersion correction and without correction

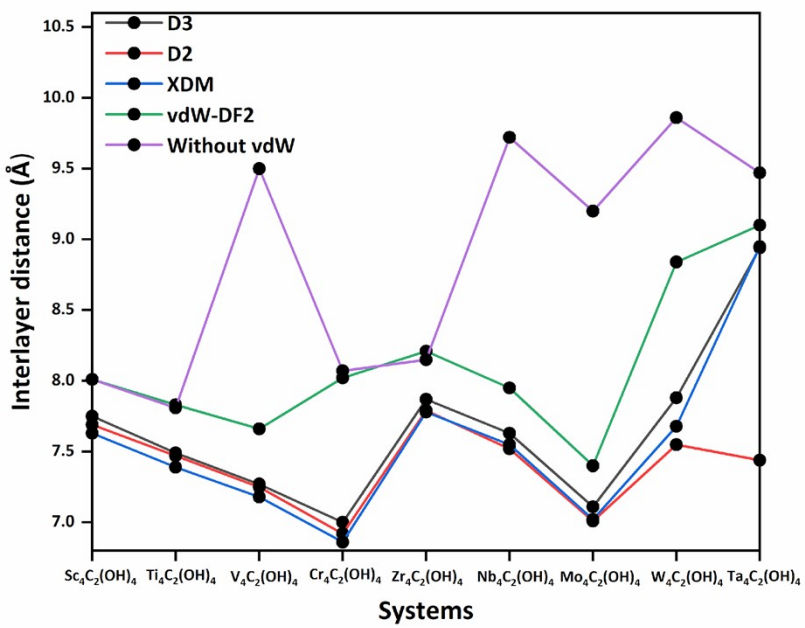

Figure S4 Interlayer distance values of 9 different hydroxyl terminated MXenes calculated with 4 different dispersion correction and without correction

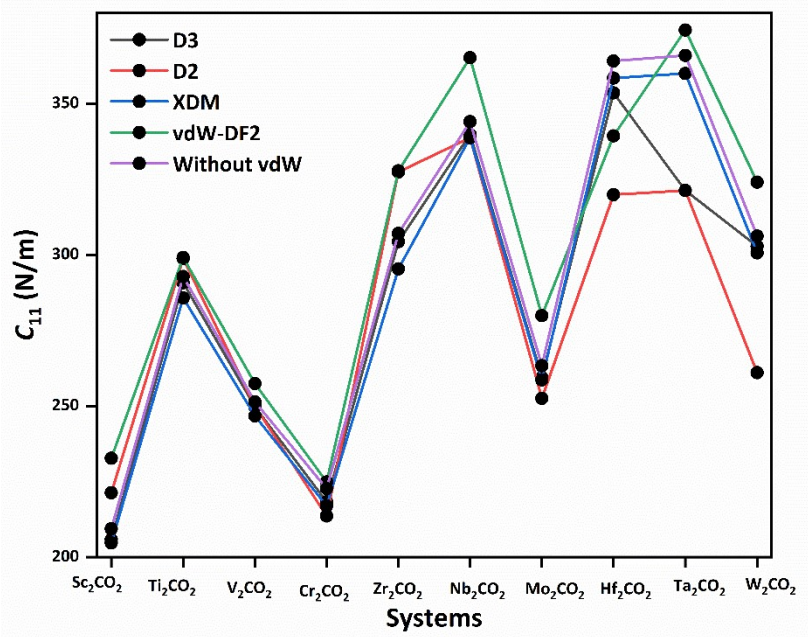

Figure S5 C_{11} elastic constant values of 10 different oxygen terminated MXenes calculated with 4 different dispersion correction and without correction

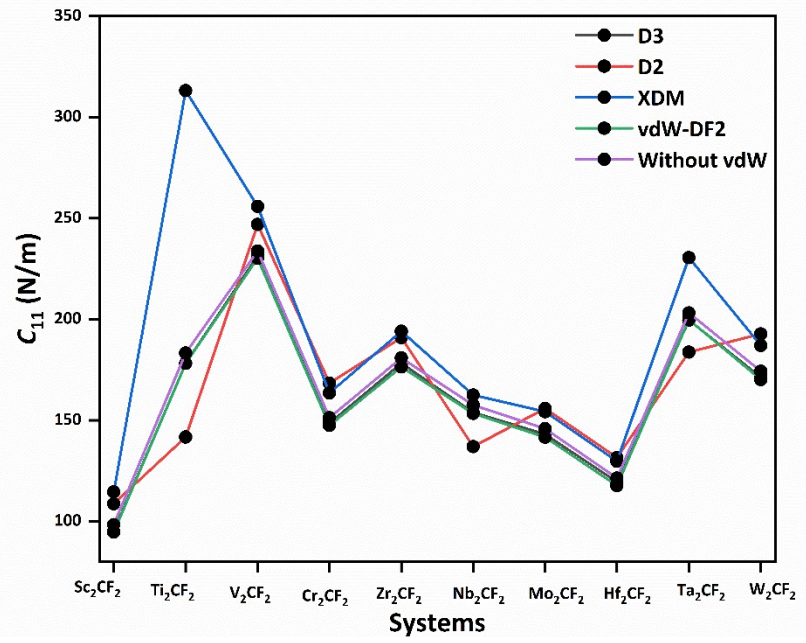

Figure S6 C_{11} elastic constant values of 10 different fluorine terminated MXenes calculated with 4 different dispersion correction and without correction

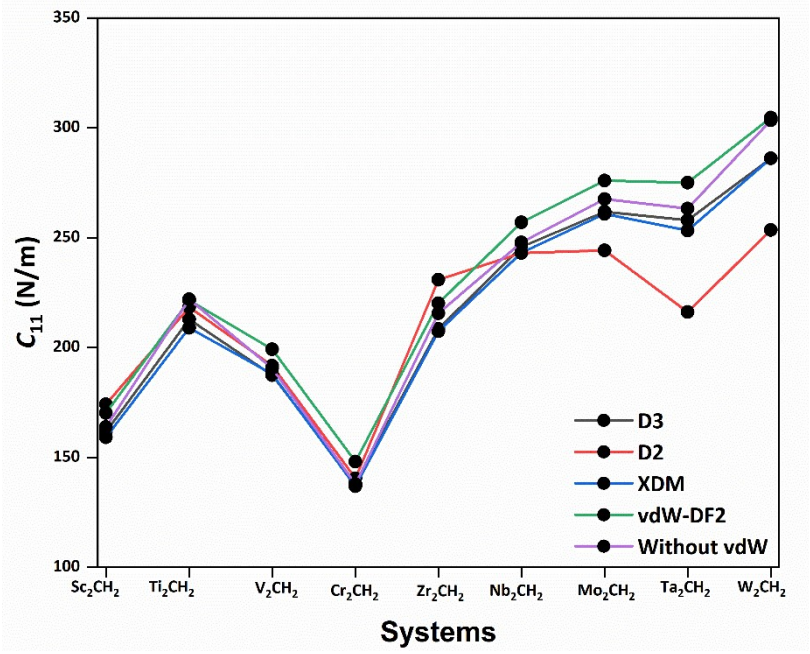

Figure S7 C_{11} elastic constant values of 9 different hydrogen terminated MXenes calculated with 4 different dispersion correction and without correction

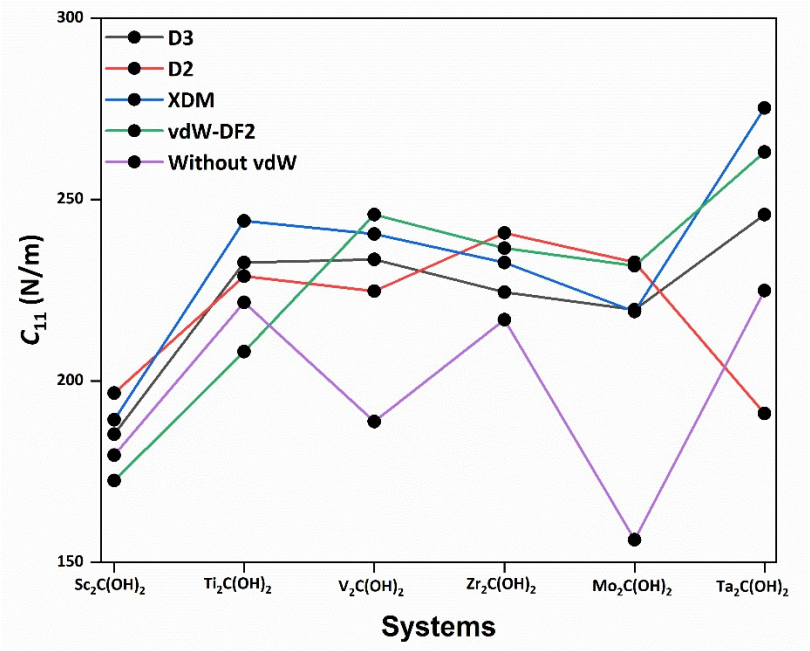

Figure S8 C_{11} elastic constant values of 6 different hydroxyl terminated MXenes calculated with 4 different dispersion correction and without correction

Table S1 Calculated intralayer bond distances for monolayer MXenes (M_2CX_T) obtained with the PBE + D3 dispersion corrections. Listed are the average M–C and M–X (X = O, F, H, OH) bond lengths (Å) for each metal (M = Sc, Ti, V, Cr, Zr, Nb, Mo, Hf, Ta, W) and termination

Metal	Termination	Bond distances (Å)	
		Metal-Carbon	Metal-Termination
Sc	O	2.51	2.01
Sc	H	2.26	2.14
Sc	F	2.27	2.20
Sc	OH	2.70	2.26
Ti	O	2.18	1.96
Ti	H	2.03	2.00
Ti	F	2.03	2.15
Ti	OH	2.17	2.10
V	O	2.04	1.95
V	H	1.99	1.92
V	F	2.00	2.14
V	OH	2.01	2.14

Cr	O	2.02	1.91
Cr	H	1.95	1.87
Cr	F	1.96	2.14
Cr	OH	1.96	2.13
Zr	O	2.36	2.12
Zr	H	2.27	2.16
Zr	F	2.26	2.32
Zr	OH	2.27	2.34
Nb	O	2.19	2.09
Nb	H	2.16	2.06
Nb	F	2.15	2.30
Nb	OH	2.13	2.29
Mo	O	2.10	2.10
Mo	H	2.12	1.98
Mo	F	2.11	2.30
Mo	OH	2.30	2.29
Hf	H	2.41	2.12

Hf	F	2.23	2.31
Hf	OH	2.23	2.32
Ta	O	2.18	2.10
Ta	H	2.15	2.04
Ta	F	2.14	2.31
Ta	OH	2.15	2.29
W	O	2.10	2.12
W	F	2.11	2.30
W	OH	2.11	2.31