Electronic Supplementary Information (ESI)

Tailoring Linear and Nonlinear Optical Properties of 2D Sc_2C MXenes via Surface Termination Modulation

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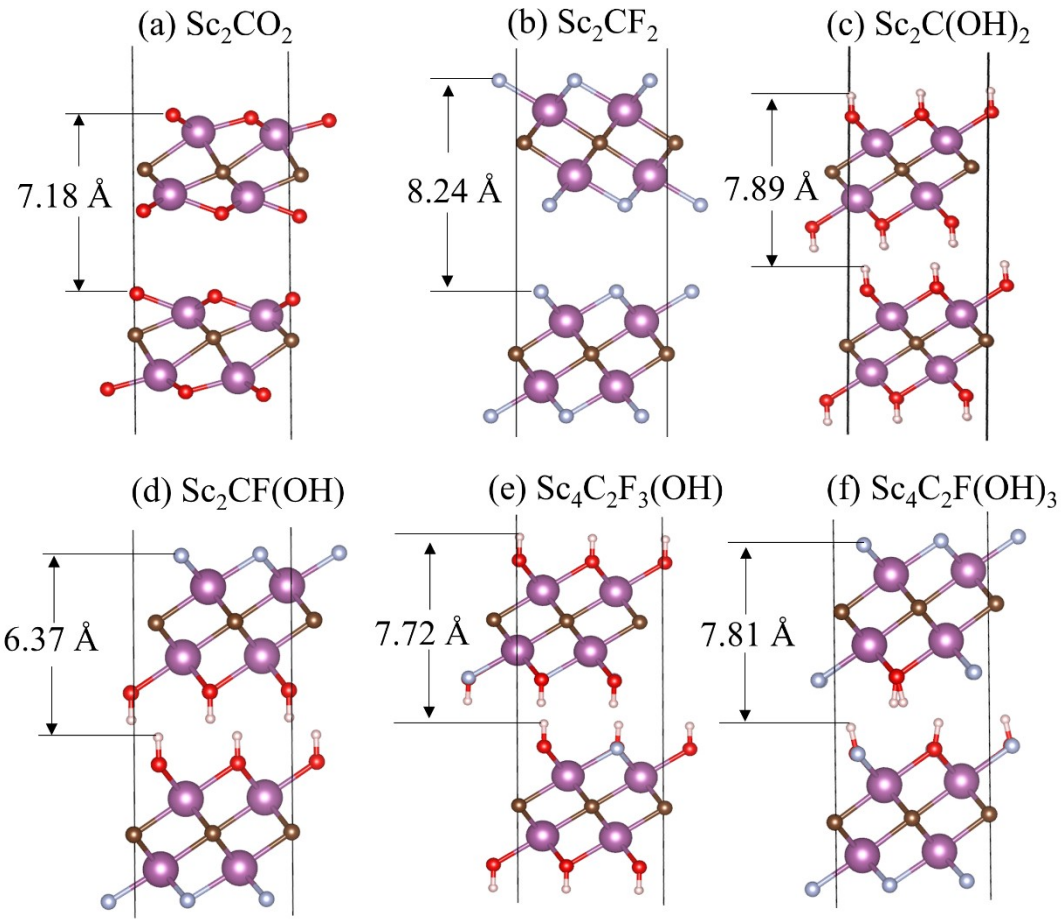

Figure S1. Bilayer model of functionalized Sc-based MXenes.

Table S1 The static SHG coefficients of Sc_2CO_2 in unit of pm/V.

d_{xy}	**1**	**2**	**3**	**4**	**5**	**6**
1	31.801	31.792	0	0	17.491	0
2	0	0	0	17.493	0	31.792
3	17.491	17.493	4.430	0	0	0

Table S2 The static SHG coefficients of Sc_2CF_2 in unit of pm/V.

d_{xy}	**1**	**2**	**3**	**4**	**5**	**6**
1	138.848	138.761	0	0	53.749	0
2	0	0.043	0	53.781	0	138.761
3	53.749	53.781	14.155	0	0	0

Table S3 The static SHG coefficients of $Sc_2C(OH)_2$ in unit of pm/V.

d_{xy}	**1**	**2**	**3**	**4**	**5**	**6**
1	191.565	191.384	0.143	0.042	119.018	0.083
2	0.083	0.074	0.070	118.74	0.042	191.384

				3		
3	119.018	118.743	93.065	0.070	0.143	0.042

Table S4 The static SHG coefficients of $Sc_2CF(OH)$ in unit of pm/V.

d_{xy}	**1**	**2**	**3**	**4**	**5**	**6**
1	171.582	171.675	0	0	66.772	0.089
2	0.089	0.054	0	66.777	0	171.675
3	66.772	66.777	86.769	0	0	0

Table S5 The static SHG coefficients of $Sc_4C_2F_3(OH)$ in unit of pm/V.

d_{xy}	**1**	**2**	**3**	**4**	**5**	**6**
1	146.184	149.429	0.029	0.185	50.470	1.492
2	1.423	4.205	0.050	50.717	0.185	149.429
3	50.470	50.717	23.081	0.050	0.029	0.185

Table S6 The static SHG coefficients of $Sc_4C_2F(OH)_3$ in unit of pm/V.

d_{xy}	**1**	**2**	**3**	**4**	**5**	**6**
1	180.782	185.008	0.101	0.541	56.550	1.721
2	1.721	5.455	0.183	57.106	0.541	185.008
3	56.550	57.106	84.290	0.183	0.101	0.541