Electronic supplementary information

Computational Studies on Structural and Electronic Properties of Functionalized MXene Monolayers and Nanotubes

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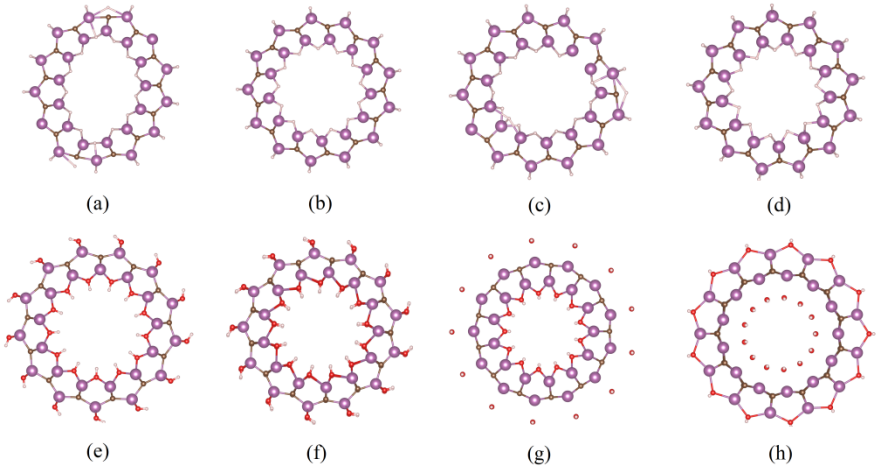

Figure S1. Atomic structures of (13,0) zigzag Sc_2CH_2 and $Sc_2C(OH)_2$ nanotubes rolled from A/Sc_2C/A, B/Sc_2C/B, and A/Sc_2C/B layers, respectively.

Table S1. Relative total energies ΔE (kal/mol/formula) for the most stable zigzag nanotubes and armchair nanotubes for Sc_2CH_2 and $Sc_2C(OH)_2$, respectively.

	ΔE (kal/mol/formula)
$(10,10)^{H}$	0
$(9,9)^{H}$	0.659
$(8,8)^{H}$	2.084
$(13,0)^{H}$	7.867
$(10,10)^{OH}$	0
$(9,9)^{OH}$	1.724
$(8,8)^{OH}$	4.495
$(13,0)^{OH}$	15.469

Table S2. Lattice parameters a (Å), length of Sc-X bond (X = H for Sc_2CH_2 or O for $Sc_2C(OH)_2$ and Sc_2CO_2) (Å), length of Sc-C bond (Å) from DFT, as well as the absolute value of fractional error between DFTB and DFT E_a, E_x and E_C.

System	a (Å)	E_a	Sc-X (Å)	E_X	Sc-C (Å)	E_C
Sc_2C	3.225	4.4%	/	/	2.221	1.7%
$A/Sc_2C/A^{(H)}$	3.233	1.1%	2.124	0.5%	2.241	0.8%
$A/Sc_2C/A^{(OH)}$	3.227	0.7%	2.216	2.2%	2.244	0.4%
$A/Sc_2C/B^{(O)}$	3.431	2.8%	2.081/2.098	0.2%/0.2%	2.530/2.201	4.4%/1.2%

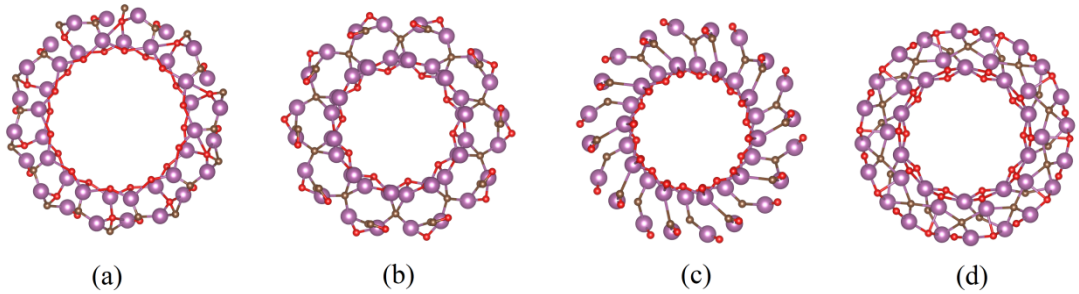

Figure S2. Atomic structures of (10,10) armchair Sc_2CO_2 nanotubes rolled from A/Sc_2C/A, B/Sc_2C/B, and A/Sc_2C/B layers, respectively.

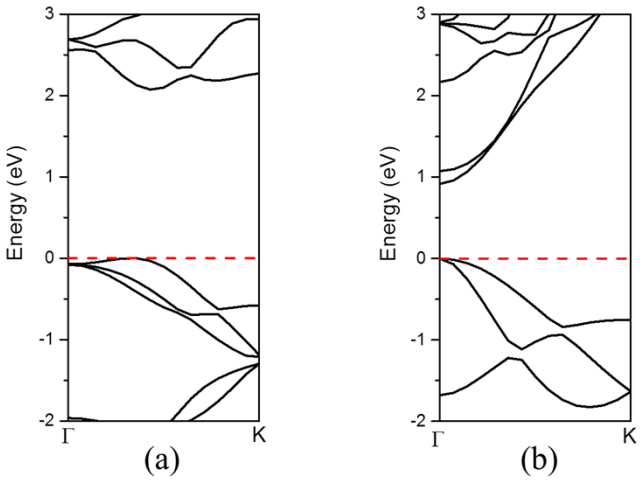

Figure S3. Band structures near Fermi level for the corresponding Sc_2CH_2 (a) and $Sc_2C(OH)_2$ (b) monolayers along direction b, respectively.