Supplementary information

Unlocking the Sensing and Scavenging Potential of Sc_2CO_2 and Sc_2CO_2/ TMD Heterostructures for Phosgene Detection

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Table S1: The atomic positions of each atom of the unit cell structures of Fig 1 of the original manuscript. Data is presented in fractional coordinates.

Struct_1			
Atom	**x**	**y**	**z**
Sc_1	0.666666687	0.333333343	0.622142017
Sc_2	0.333333343	0.666666687	0.377857983
C	0	0	0.5
O_1	0.666666687	0.333333343	0.212495565
O_2	0.333333343	0.666666687	0.787504435
Struct_2			
Atom	**x**	**y**	**z**
Sc_1	0.666666806	0.333333433	0.622141957
Sc_2	0.333333433	0.666666865	0.377857953
C	0	0	0.5
O_1	0	0	0.21249561
O_2	0	0	0.787504435
Struct_3			
Atom	**x**	**y**	**z**
Sc_1	0.666666687	0.333333343	0.622142017
Sc_2	0.333333343	0.666666687	0.377857983
C	0	0	0.5
O_1	0.666666687	0.333333343	0.212495551
O_2	0	0	0.787504435
Struct_4			
Atom	**x**	**y**	**z**
Sc_1	0.666666687	0.333333343	0.622142017
Sc_2	0.333333343	0.666666687	0.377857983
C	0	0	0.5
O_1	0.666666687	0.333333343	0.787504435
O_2	0.333333343	0.666666687	0.212495551

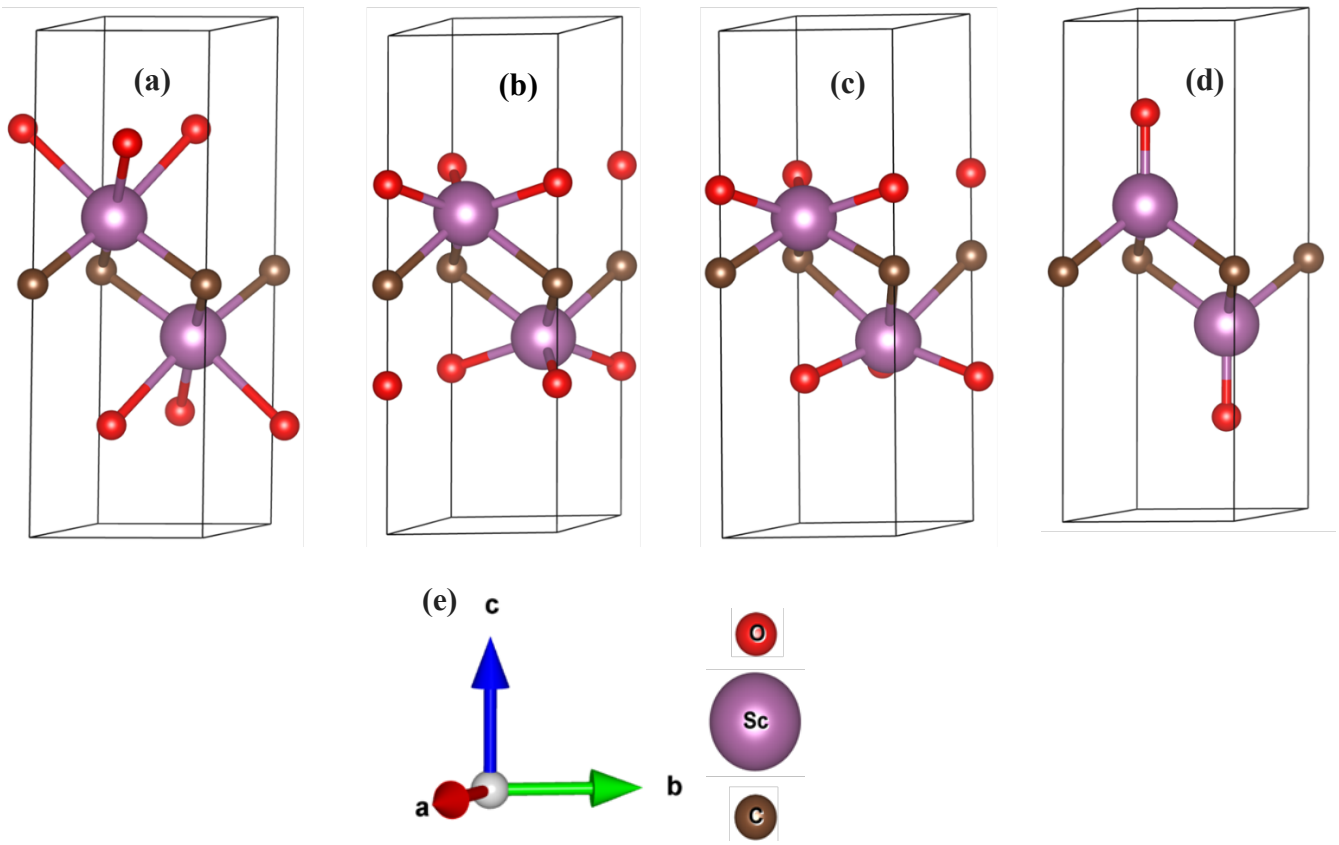

Figure S1. 3D representation of unit cell structures of different models of Sc_2CO_2 (a) Struct_1, (b) Struct_2, (c) Struct_3, and (d) Struct_4 (e) Lattice direction

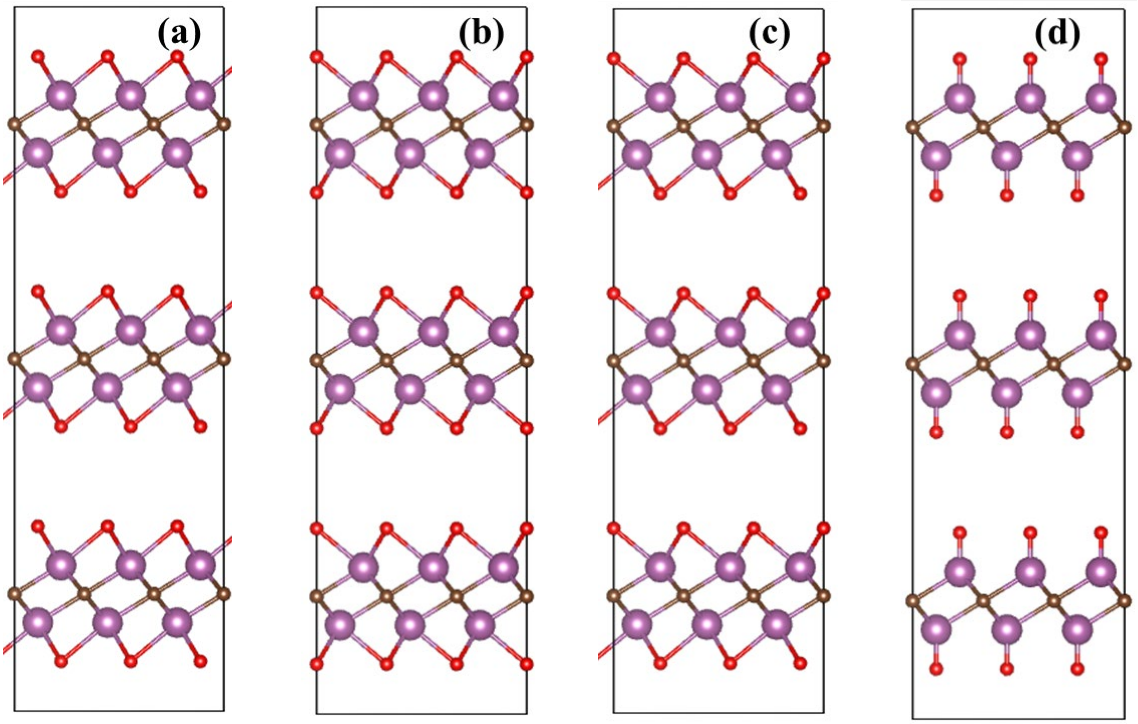

Figure S2. Supercell structures of different models of Sc_2CO_2 (a) Struct_1, (b) Struct_2, (c) Struct_3, and (d) Struct_4

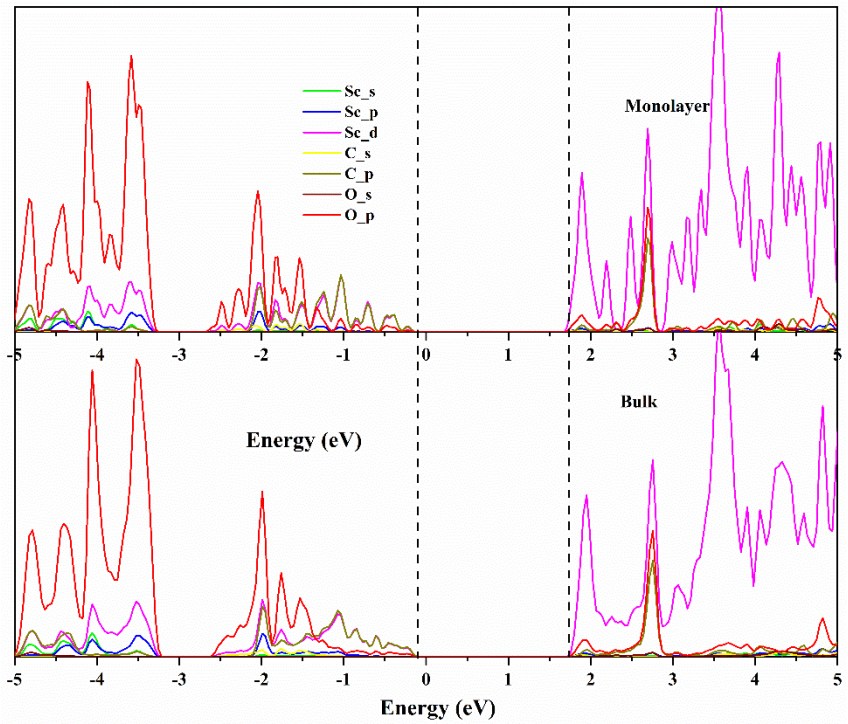

Figure S3. Partial DOS spectra of bulk and monolayer

Table S2: The calculated distance (d) of gas from MXene surface, adsorption energy (E_{ad}) without vdW correction, charge transfer (Δq), recovery time (τ) at 298 K and 373K, of CO, NO, CH_4, H_2S, $COCl_2$, O_2, and N_2 after interaction with Sc_2CO_2

Model	d (Å)	E_{ad} (eV)	Δq (e)	τ (s)/298K	τ (s)/373K
Sc_2CO_2	-	-	-	-	-
$Sc_2CO_2 + O_2$	1.6	-1.04	0.067	3.73×10^{5}	109.8
$Sc_2CO_2 + CO$	2.98	-1.05	-0.006	5.5×10^{5}	148
$Sc_2CO_2 + N_2$	1.5	-1.06	0.007	8.13×10^{5}	204
$Sc_2CO_2 + NO$	2.49	-1.16	0.034	5.13×10^{7}	5590
$Sc_2CO_2 + CH_4$	2.53	-1.32	0.049	2.68×10^{10}	8.3×10^{5}
$Sc_2CO_2 + H_2S$	2.14	-1.75	0.175	5.44×10^{17}	5.7×10^{11}
$Sc_2CO_2 + COCl_2$	3.00	-1.97	-0.005	2.95×10^{21}	5.48×10^{14}
WSe_2_Sc_2CO_2	-	-	-	-	-
WSe_2_Sc_2CO_2+$COCl_2$	1.6	-1.905	1.867	2.33×10^{20}	7.23×10^{13}
$MoSe_2$_Sc_2CO_2	-	-	-	-	-
$MoSe_2$_Sc_2CO_2+$COCl_2$	1.8	-1.915	1.880	3.44×10^{20}	9.83×10^{13}