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Supplementary Information

Amine functionalized stable Nb_2CT_x MXene towards room temperature ultrasensitive NO_2 gas sensor

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FTIR:

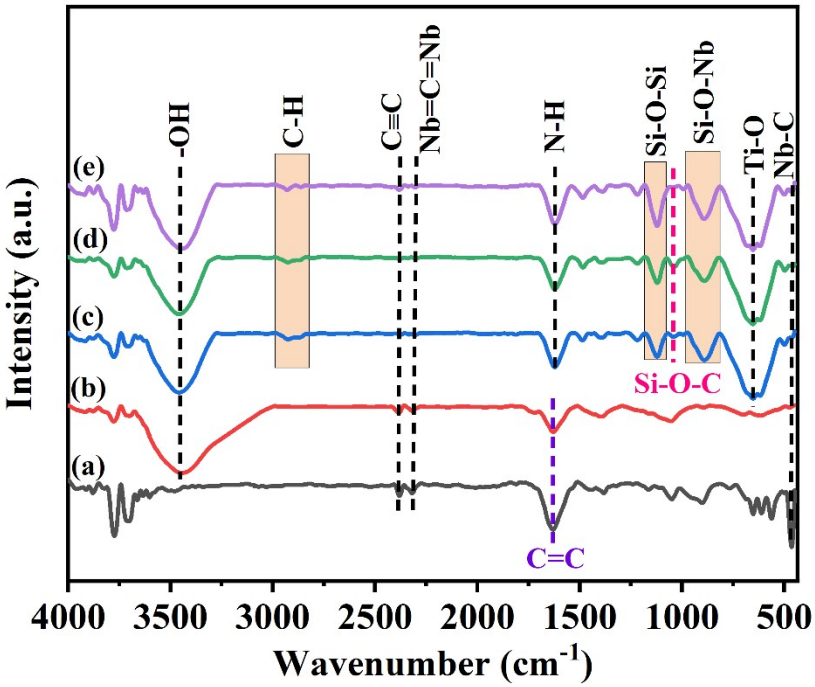

Figure S1. FTIR of Nb_2AlC MAX Phase(a), Nb_2C MXene (b), Nb_2C-0.1 APTES (c), Nb_2C-0.2 APTES (d), Nb_2C-0.3 APTES (e).

XPS:

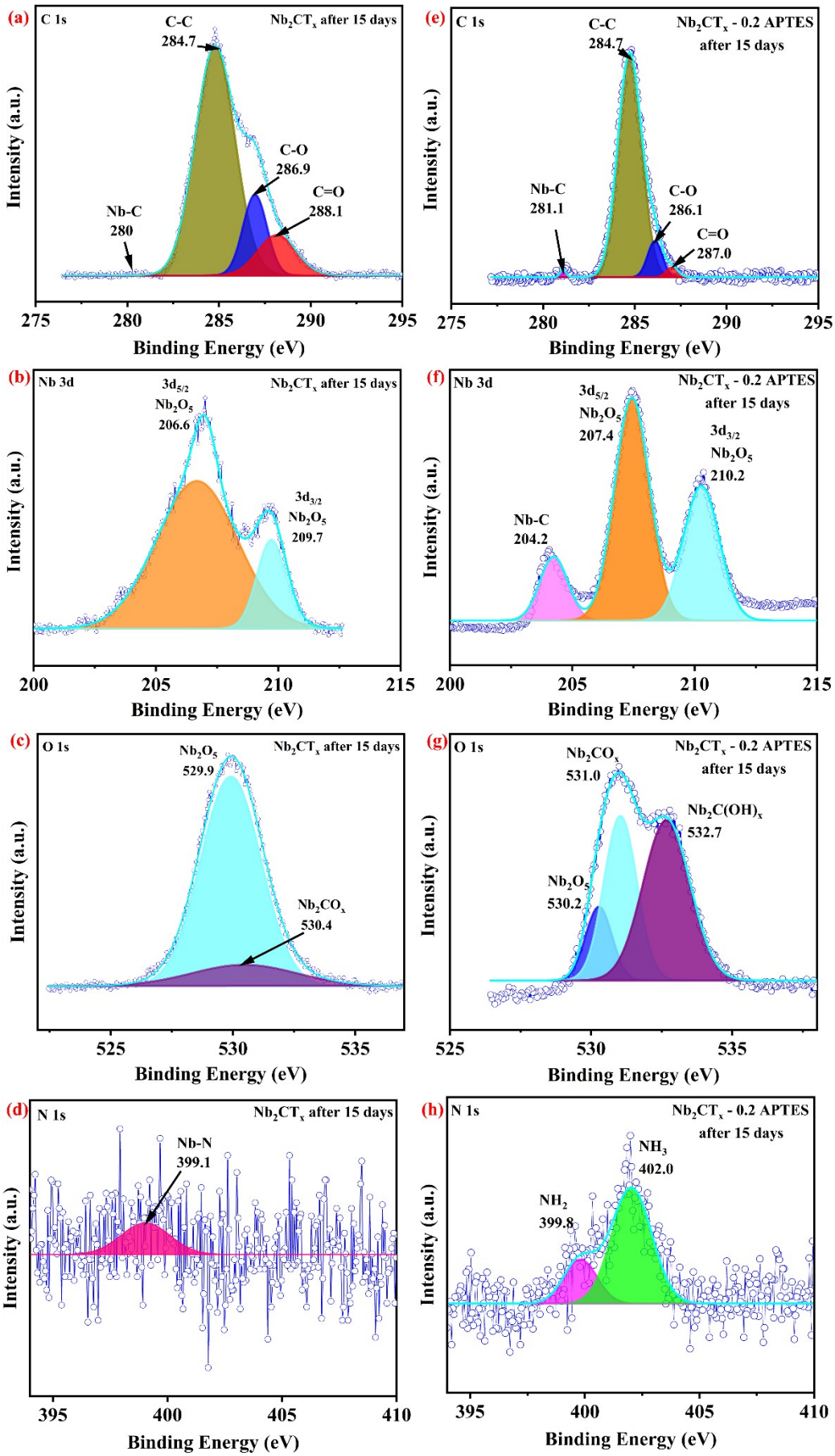
(a)
C 1s
Nb2CTx after 15 days
C-C
284.7
C-O
286.9
C=O
288.1
Nb-C
280
Intensity (a.u.)
Binding Energy (eV)
(e)
C 1s
Nb2CTx - 0.2 APTES
after 15 days
C-C
284.7
Nb-C
281.1
C-O
286.1
C=O
287.0
(b)
Nb 3d
Nb2CTx after 15 days
3d5/2
Nb2O5
206.6
3d3/2
Nb2O5
209.7
(f)
Nb 3d
Nb2CTx - 0.2 APTES
after 15 days
3d5/2
Nb2O5
207.4
3d3/2
Nb2O5
210.2
Nb-C
204.2
(c)
O 1s
Nb2CTx after 15 days
Nb2O5
529.9
Nb2COx
530.4
(g)
O 1s
Nb2CTx - 0.2 APTES
after 15 days
Nb2COx
531.0
Nb2C(OH)x
532.7
Nb2O5
530.2
(d)
N 1s
Nb2CTx after 15 days
Nb-N
399.1
(h)
N 1s
Nb2CTx - 0.2 APTES
after 15 days
NH3
402.0
NH2
399.8

Figure S2. XPS results of Nb_2CT_x MXene (a-d) and Nb_2CT_x – 0.2 APTES MXene (e-h) after 15 days

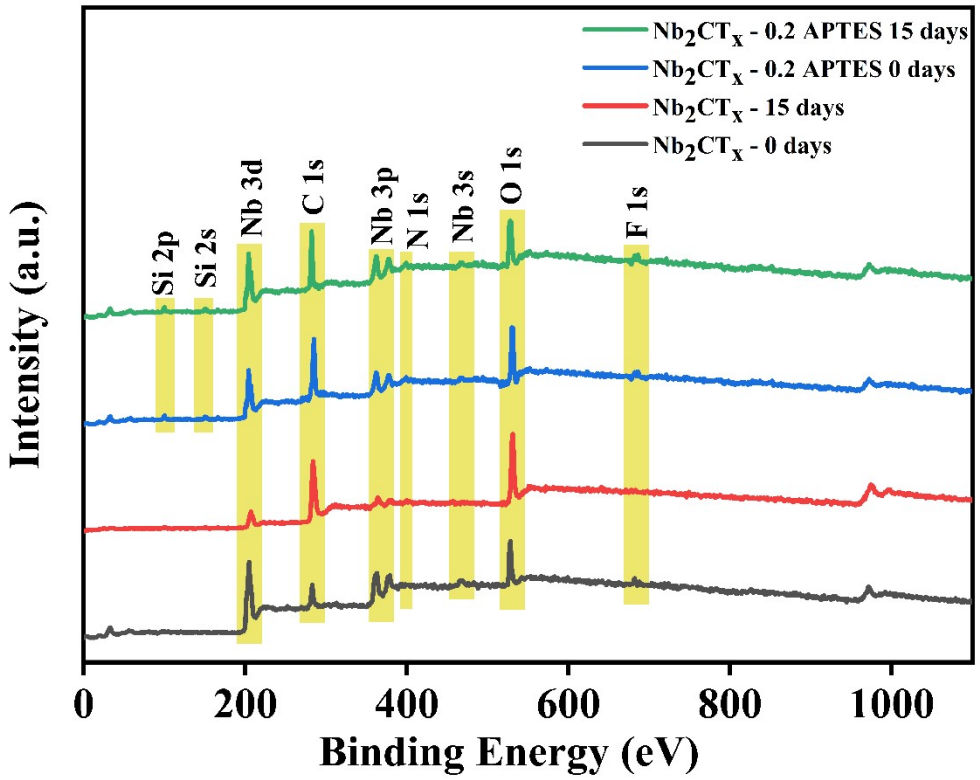

Figure S3. XPS full spectrum of Nb_2CT_x MXene and Nb_2CT_x – 0.2 APTES MXene before and after 15 days

Table S1. Atomic concentration table of prepared samples

Material / Elements	C	Nb	O	N	F	Si
Nb_2CT_x 0 days	42.25	21.39	31.94	3.64	0.78	NIL
Nb_2CT_x 15 days	68.2	1.81	28.74	1.25	0	NIL
Nb_2CT_x – 0.2 APTES 0 days	47.41	8.74	28.65	9.51	1.12	4.57
Nb_2CT_x – 0.2 APTES 15 days	48.05	9.28	27.71	9.06	1.26	4.64

FE-SEM of Nb_2ALC MAX Phase:

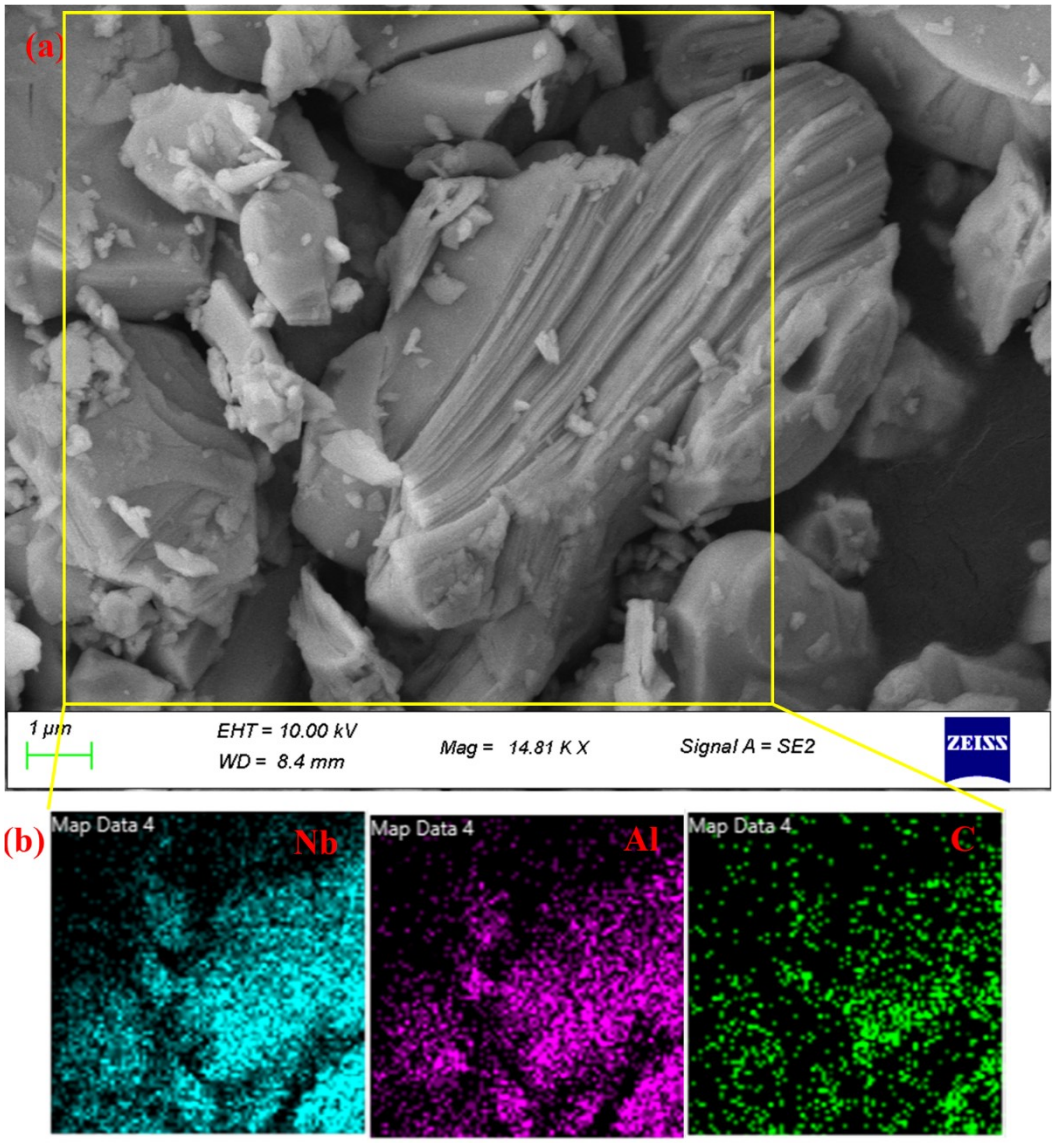

Figure S4. (a) FE-SEM image of Nb_2AlC MAX phase and (b) elemental mapping of Nb_2AlC MAX phase

HR-TEM:

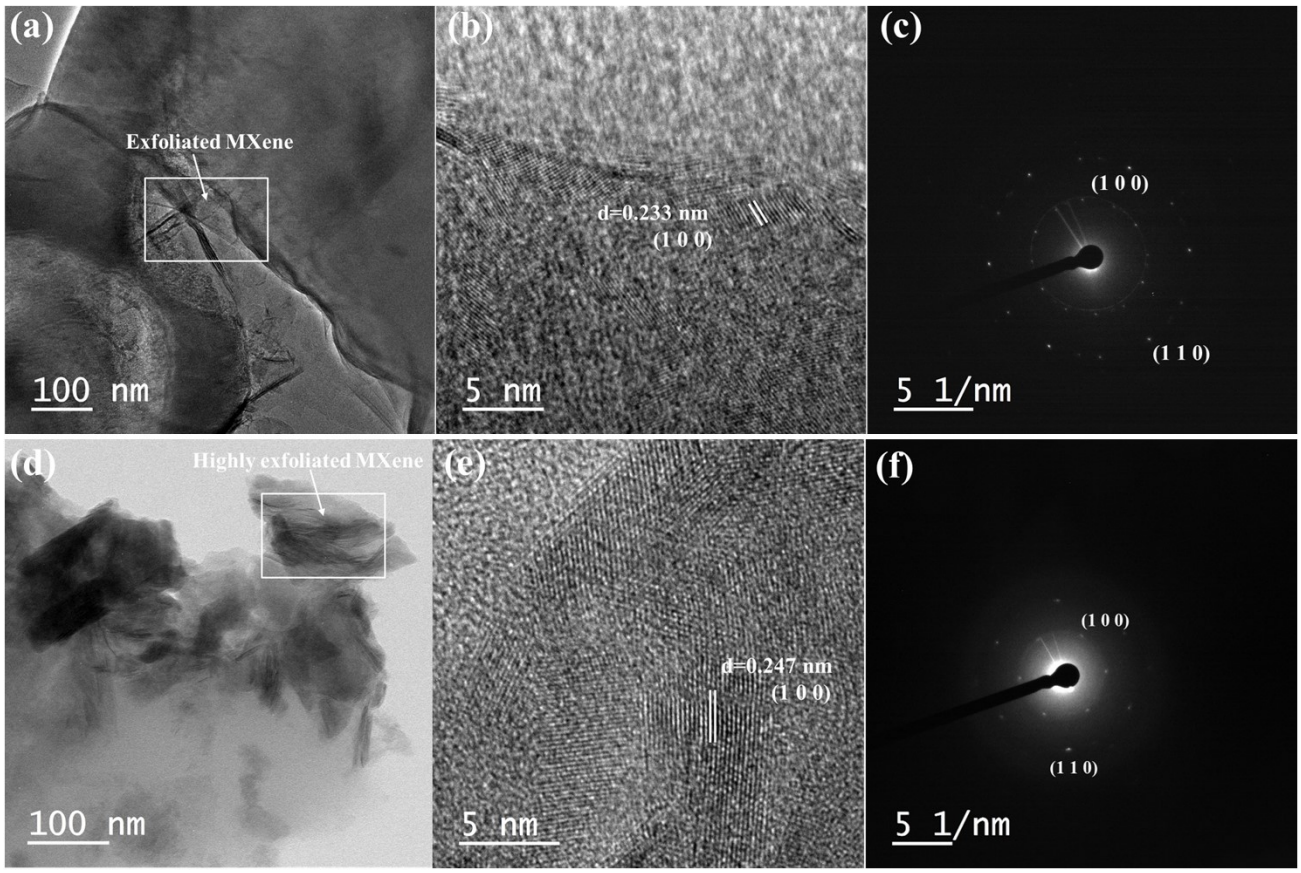

Figure S5. (a-c) TEM, HR-TEM and SAED pattern of pristine Nb_2CT_x MXene, and (d-f) TEM, HR-TEM and SAED pattern of pristine Nb_2CT_x – 0.2 APTES MXene

BET Analysis of prepared materials:

Table S2. BET analysis results of pristine Nb_2CT_x and Nb_2CT_x – 0.2 APTES (at 273 K)

Sample	Pore width (nm)	Surface area (m^2/g)	Pore Volume (cm^3/g)
Nb_2CT_x	3.801	40.892	0.058
Nb_2CT_x – 0.2 APTES	4.268	49.377	0.042

Zeta potential:

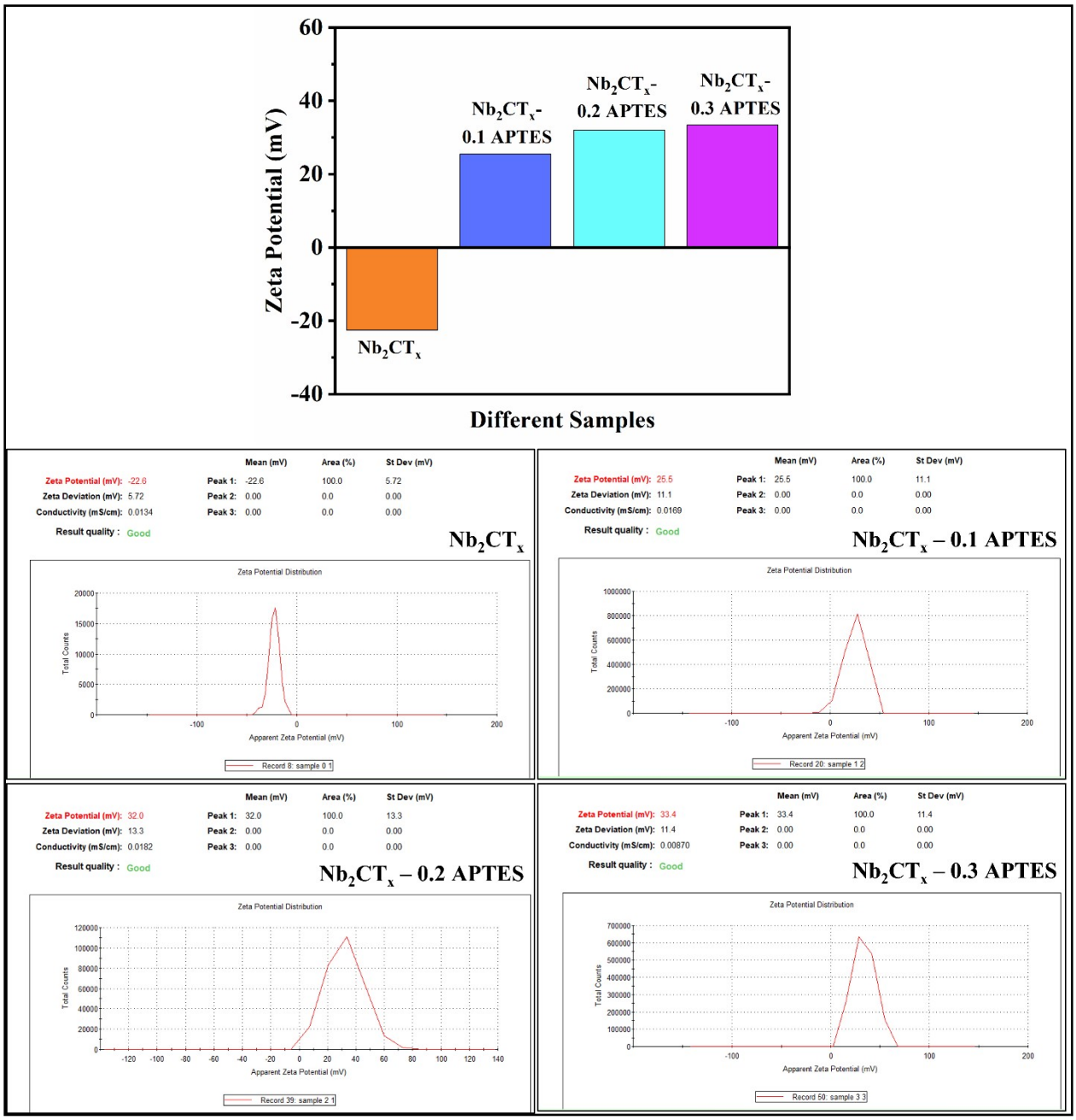

Figure S6. Zeta potential results of pristine and APTES functionalized Nb_2CT_x MXene at different concentration

UV-Vis Analysis:

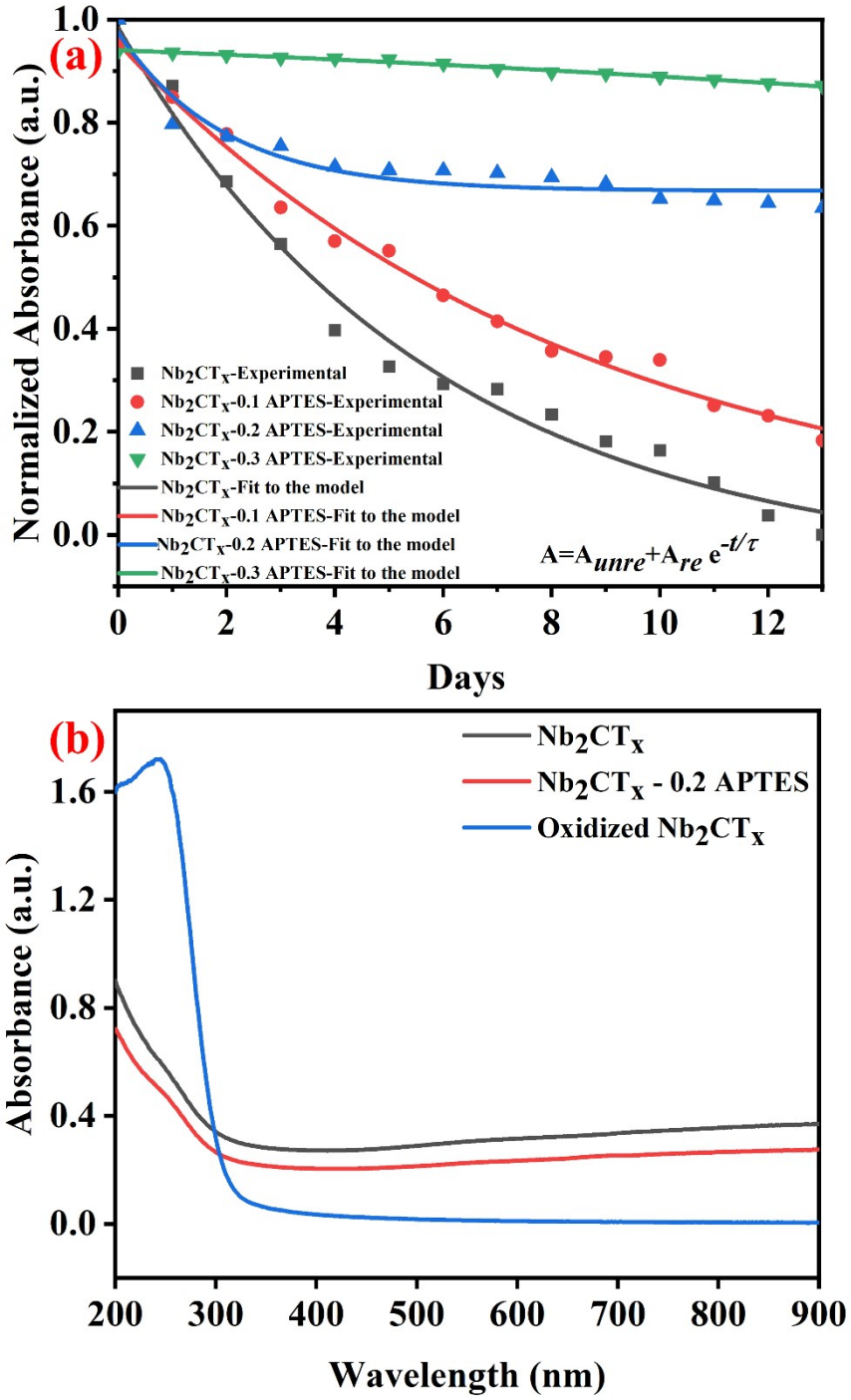

Figure S7. (a) Stability of pristine and functionalized Nb_2CT_x MXene, (b) Absorbance of MXene, Oxidized MXene and functionalized MXene

Experimental setup:

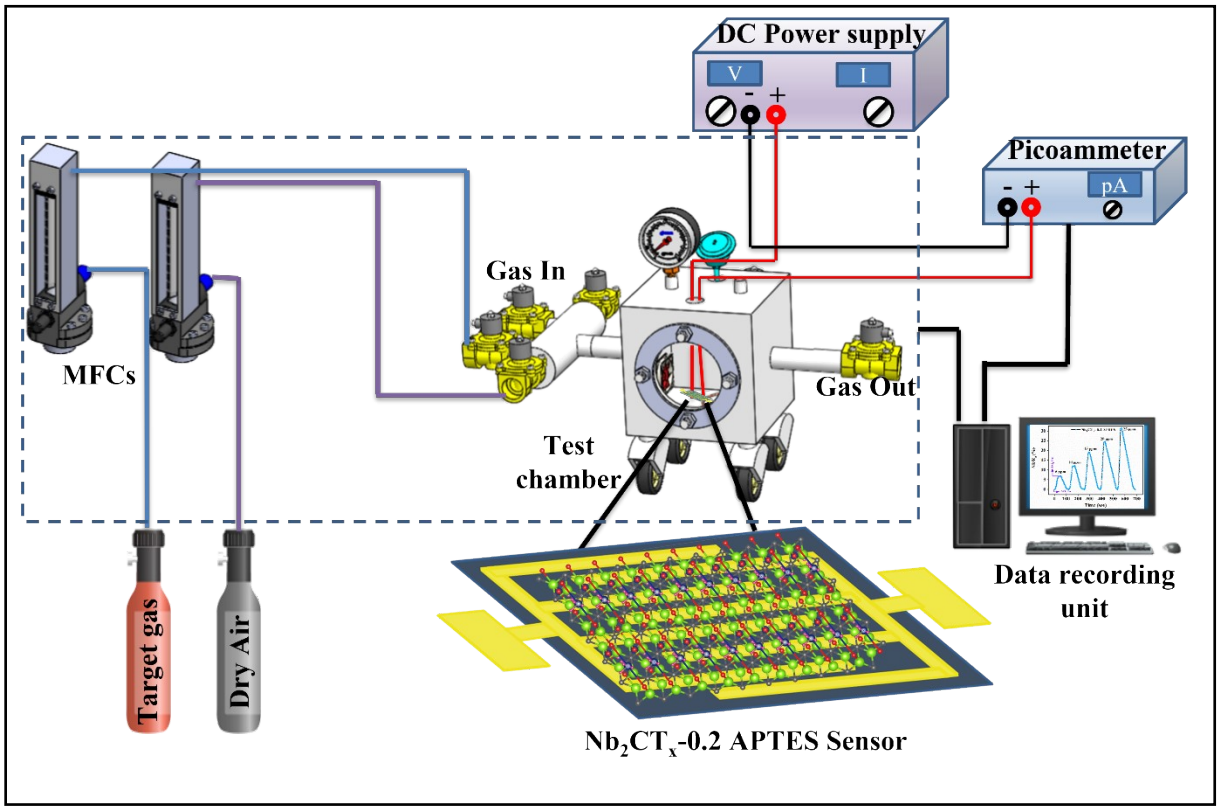

Figure S8. Schematic representation of experimental setup and fabricated sensor

I-V Characteristics:

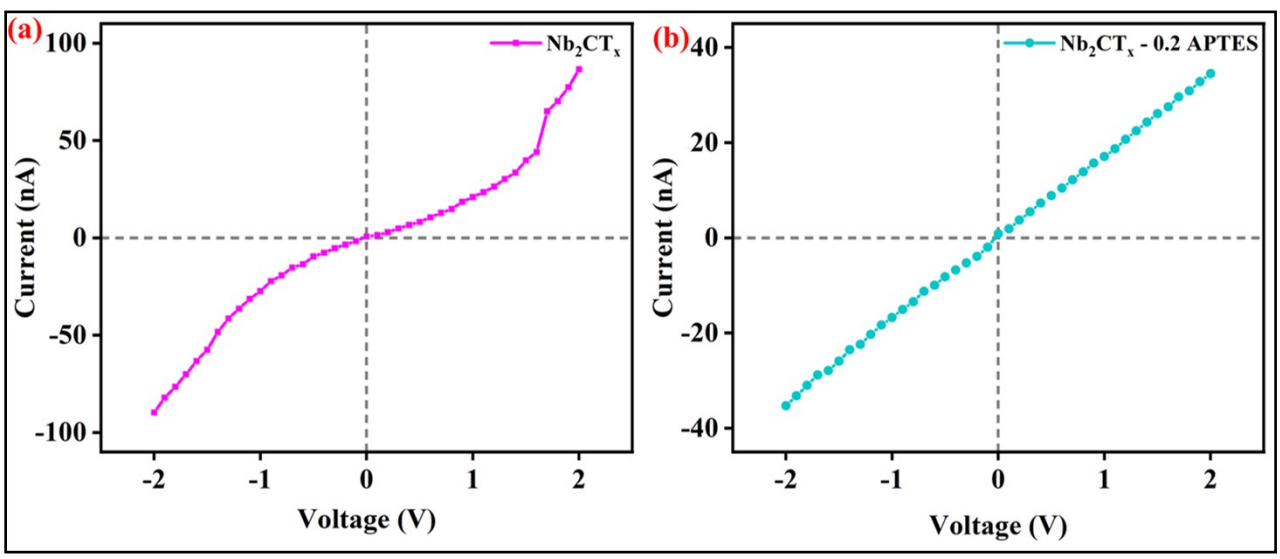

Figure S9. I-V characteristics of (a) Nb_2CT_x and (b) Nb_2CT_x – 0.2 APTES MXene based sensors

Dynamic sensing response:

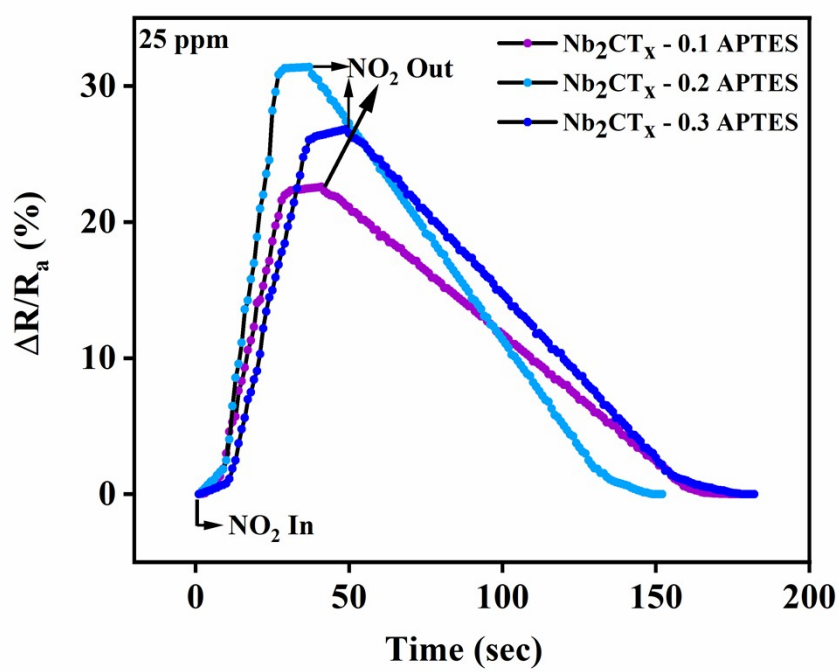

Figure S10. Dynamic sensing response of APTES functionalized Nb_2CT_x MXene at different concentration

Sensing response under different relative humidity:

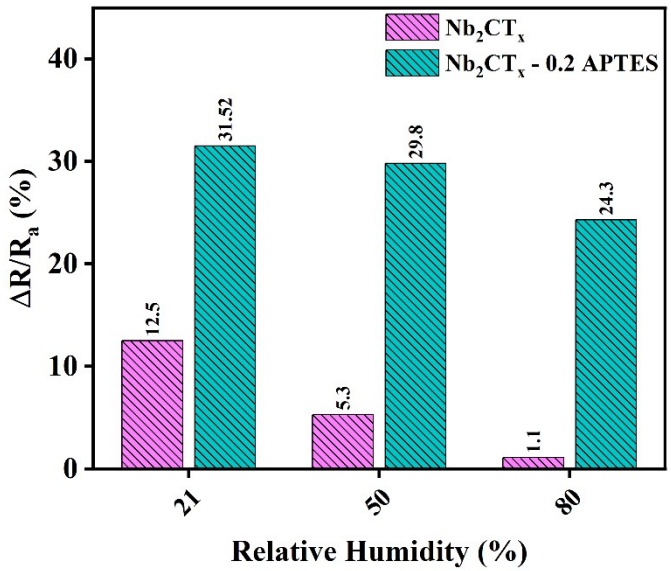

Figure S11. Sensing response of Nb_2CT_x MXene and Nb_2CT_x – 0.2 APTES MXene sensor at different relative humidity for 25 ppm of NO_2 gas

Bandgap from Tauc plot:

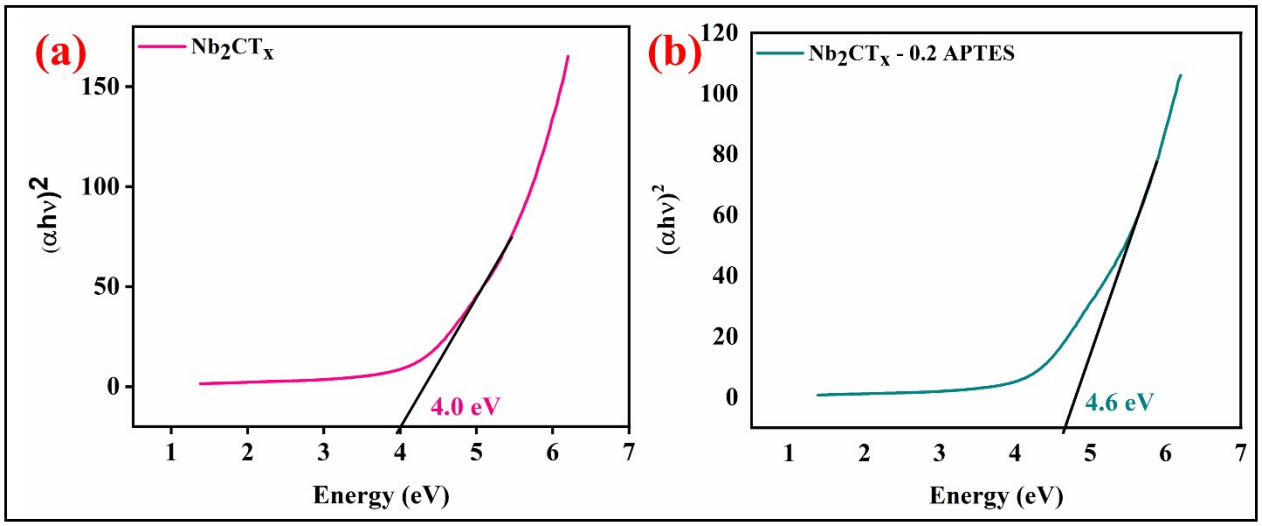

Figure S12. Tauc plot for (a) pristine Nb_2CT_x (b) APTES functionalized Nb_2CT_x MXene