Supplementary Information

Amine functionalized stable Nb$_2$CT$_x$ MXene towards room temperature ultrasensitive NO$_2$ gas sensor

 Arkoti Naveen Kumar$^1$, Kaushik Pal$^{1,2,*}$
**FTIR:**

![FTIR Spectrum](image)

**Figure S1.** FTIR of Nb$_2$AlC MAX Phase(a), Nb$_2$C MXene (b), Nb$_2$C-0.1 APTES (c), Nb$_2$C-0.2 APTES (d), Nb$_2$C-0.3 APTES (e).

**XPS:**
Figure S2. XPS results of Nb$_2$CT$_x$ MXene (a-d) and Nb$_2$CT$_x$ – 0.2 APTES MXene (e-h) after 15 days

Figure S3. XPS full spectrum of Nb$_2$CT$_x$ MXene and Nb$_2$CT$_x$ – 0.2 APTES MXene before and after 15 days

Table S1. Atomic concentration table of prepared samples

<table>
<thead>
<tr>
<th>Material</th>
<th>Elements</th>
<th>C</th>
<th>Nb</th>
<th>O</th>
<th>N</th>
<th>F</th>
<th>Si</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nb$_2$CT$_x$ 0 days</td>
<td></td>
<td>42.25</td>
<td>21.39</td>
<td>31.94</td>
<td>3.64</td>
<td>0.78</td>
<td>NIL</td>
</tr>
<tr>
<td>Nb$_2$CT$_x$ 15 days</td>
<td></td>
<td>68.2</td>
<td>1.81</td>
<td>28.74</td>
<td>1.25</td>
<td>0</td>
<td>NIL</td>
</tr>
<tr>
<td>Nb$_2$CT$_x$ – 0.2 APTES 0</td>
<td></td>
<td>47.41</td>
<td>8.74</td>
<td>28.65</td>
<td>9.51</td>
<td>1.12</td>
<td>4.57</td>
</tr>
<tr>
<td>days</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nb$_2$CT$_x$ – 0.2 APTES 15</td>
<td></td>
<td>48.05</td>
<td>9.28</td>
<td>27.71</td>
<td>9.06</td>
<td>1.26</td>
<td>4.64</td>
</tr>
<tr>
<td>days</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**FE-SEM of Nb$_2$AlC MAX Phase:**

Figure S4. (a) FE-SEM image of Nb$_2$AlC MAX phase and (b) elemental mapping of Nb$_2$AlC MAX phase
**HR-TEM:**

![HR-TEM images](image)

Figure S5. (a-c) TEM, HR-TEM and SAED pattern of pristine Nb$_2$CT$_x$ MXene, and (d-f) TEM, HR-TEM and SAED pattern of pristine Nb$_2$CT$_x$ – 0.2 APTES MXene

**BET Analysis of prepared materials:**

Table S2. BET analysis results of pristine Nb$_2$CT$_x$ and Nb$_2$CT$_x$ – 0.2 APTES (at 273 K)

<table>
<thead>
<tr>
<th>Sample</th>
<th>Pore width (nm)</th>
<th>Surface area (m$^2$/g)</th>
<th>Pore Volume (cm$^3$/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nb$_2$CT$_x$</td>
<td>3.801</td>
<td>40.892</td>
<td>0.058</td>
</tr>
<tr>
<td>Nb$_2$CT$_x$ – 0.2 APTES</td>
<td>4.268</td>
<td>49.377</td>
<td>0.042</td>
</tr>
</tbody>
</table>
Zeta potential:

Figure S6. Zeta potential results of pristine and APTES functionalized Nb$_2$CT$_x$ MXene at different concentration.
UV-Vis Analysis:

**Figure S7.** (a) Stability of pristine and functionalized Nb$_2$CT$_x$ MXene, (b) Absorbance of MXene, Oxidized MXene and functionalized MXene
**Experimental setup:**

![Experimental setup diagram](image)

*Figure S8. Schematic representation of experimental setup and fabricated sensor*

**I-V Characteristics:**

![I-V Characteristic graphs](image)

*Figure S9. I-V characteristics of (a) Nb$_2$CT$_x$ and (b) Nb$_2$CT$_x$ – 0.2 APTES MXene based sensors*
Dynamic sensing response:

Figure S10. Dynamic sensing response of APTES functionalized Nb$_2$CT$_x$ MXene at different concentration

Sensing response under different relative humidity:

Figure S11. Sensing response of Nb$_2$CT$_x$ MXene and Nb$_2$CT$_x$ – 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\(_2\)CT\(_x\) (b) APTES functionalized Nb\(_2\)CT\(_x\) MXene