Supplementary information

# In situ fabrication of NiO nanoparticles / single-layered MXene nanosheet Schottky heterojunction toward sensing xylene and formaldehyde

Xueying Song,[a] Kuikun Gu,[a] Qinwei Zhang,[a] Linhu Jin[a], Chunfeng He* and Mingzhe Zhang*[a]

[a] *State Key Laboratory of Superhard Materials, college of physics, Jilin University, Changchun 130012, People's Republic of China. Email address:* zhangmz@jlu.edu.cn, hecf@jlu.edu.cn

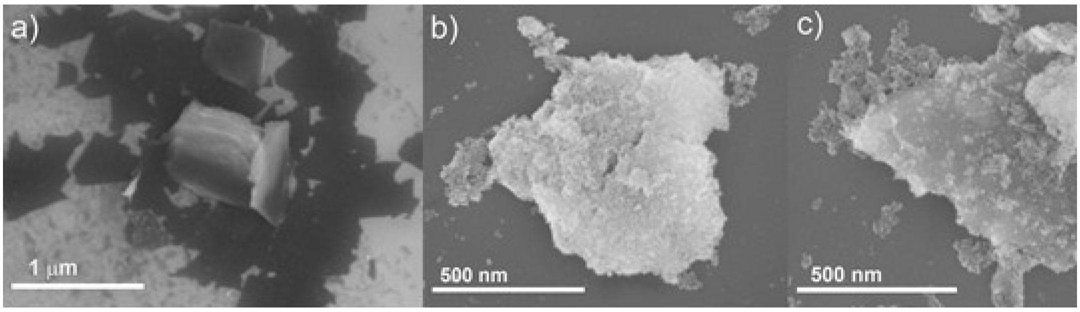



**Fig. S1** SEM image of (a) single layered MXene (b) NiO and (c) NiO-MXene.

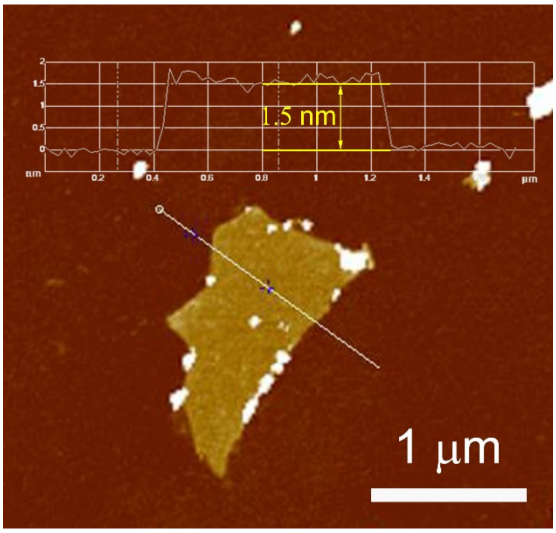



**Fig. S2** AFM of single-layer $Ti_3C_2T_x$ MXene

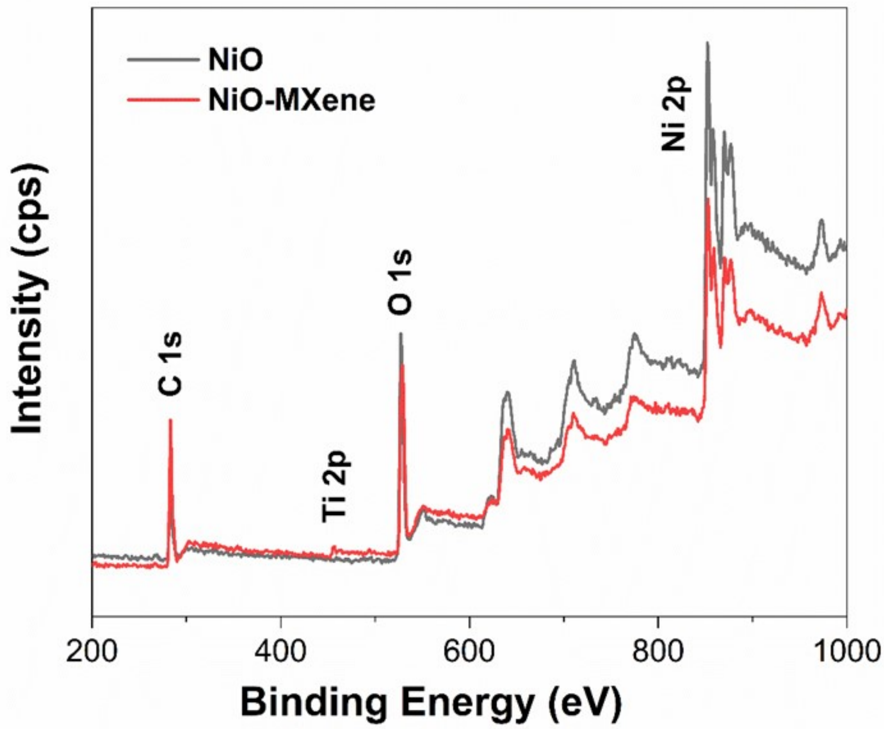



**Fig. S3** Wide XPS spectrum of pure NiO and NiO-$Ti_3C_2T_x$ MXene composites.

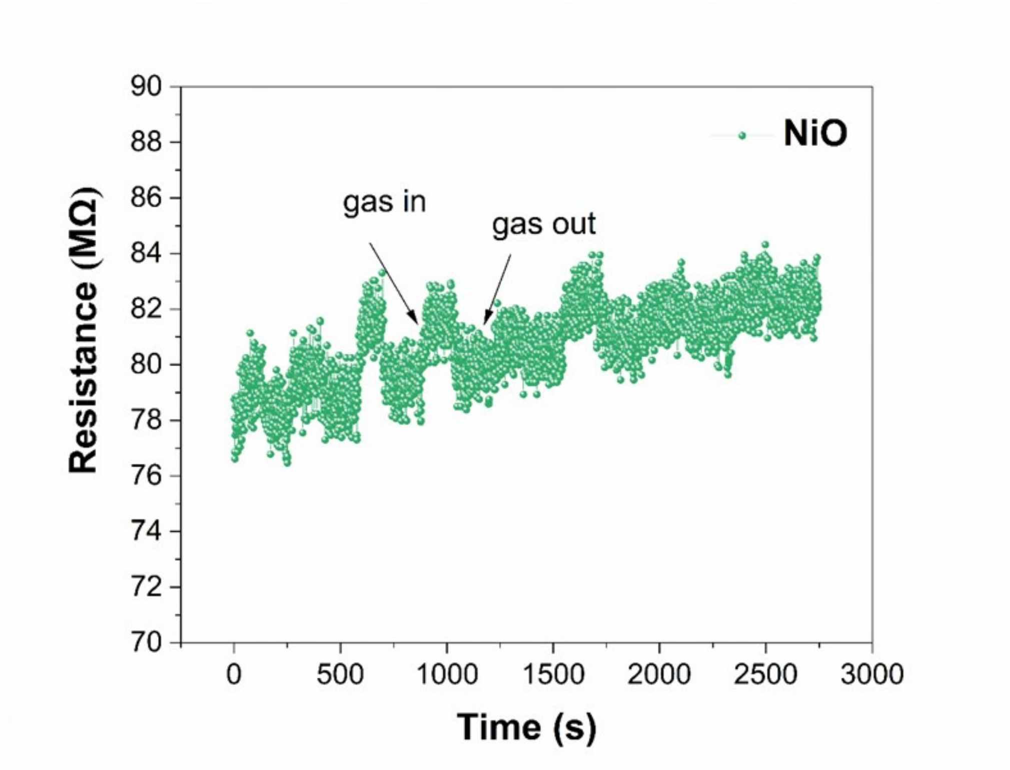



**Fig. S4** The response of pure NiO based sensor to 500 ppm xylene at room temperature.

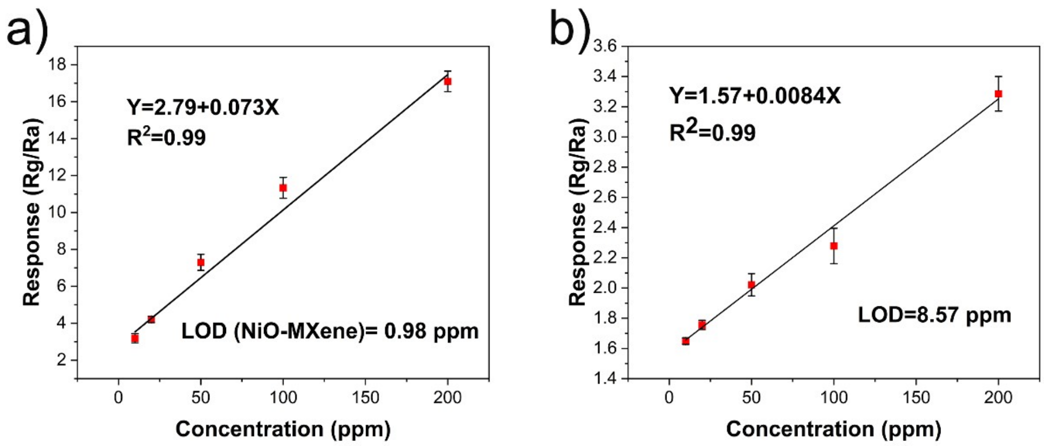



Fig. S5 (a) The linear fitting of response curve of NiO-MXene based sensors. (b) The linear fitting of response curve of NiO-MXene based sensors.

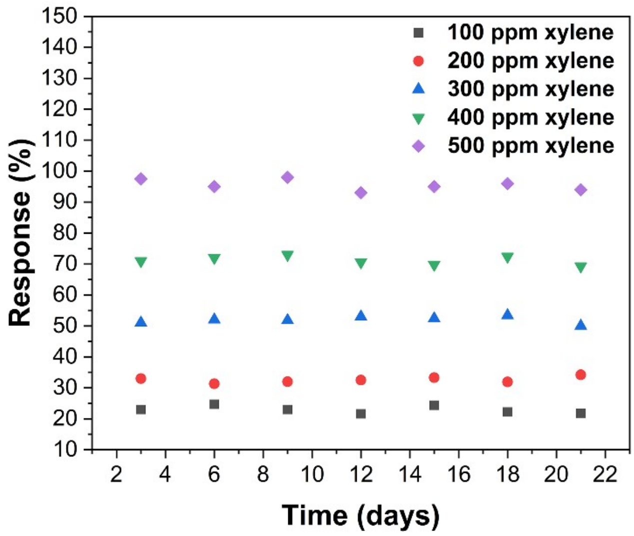



**Fig. S6** The long-term stability of NiO-MXene based sensor at room temperature to a variety of xylene concentrations

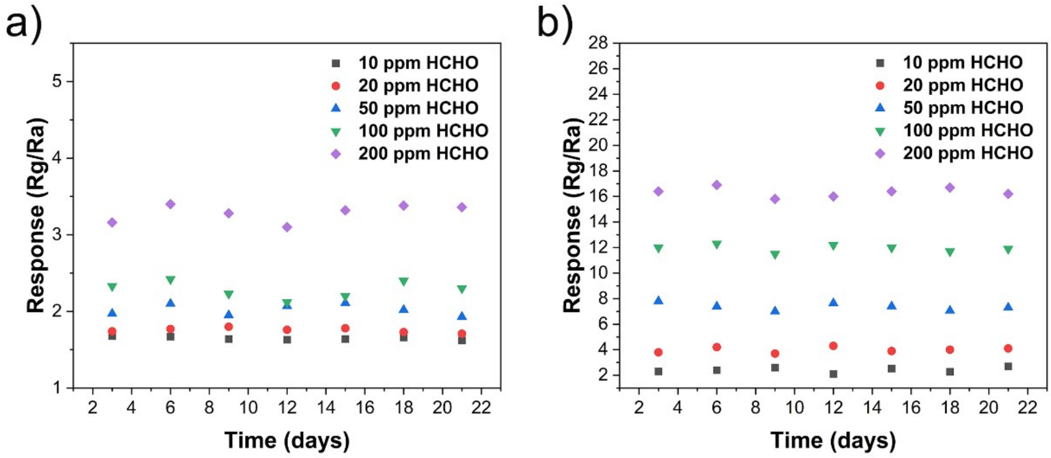



**Fig. S7** (a) The long-term stability of pure NiO based sensor at 170℃ to a variety of formaldehyde concentrations;(b) The long-term stability of NiO-MXene based sensor at 170℃ to a variety of formaldehyde concentrations.

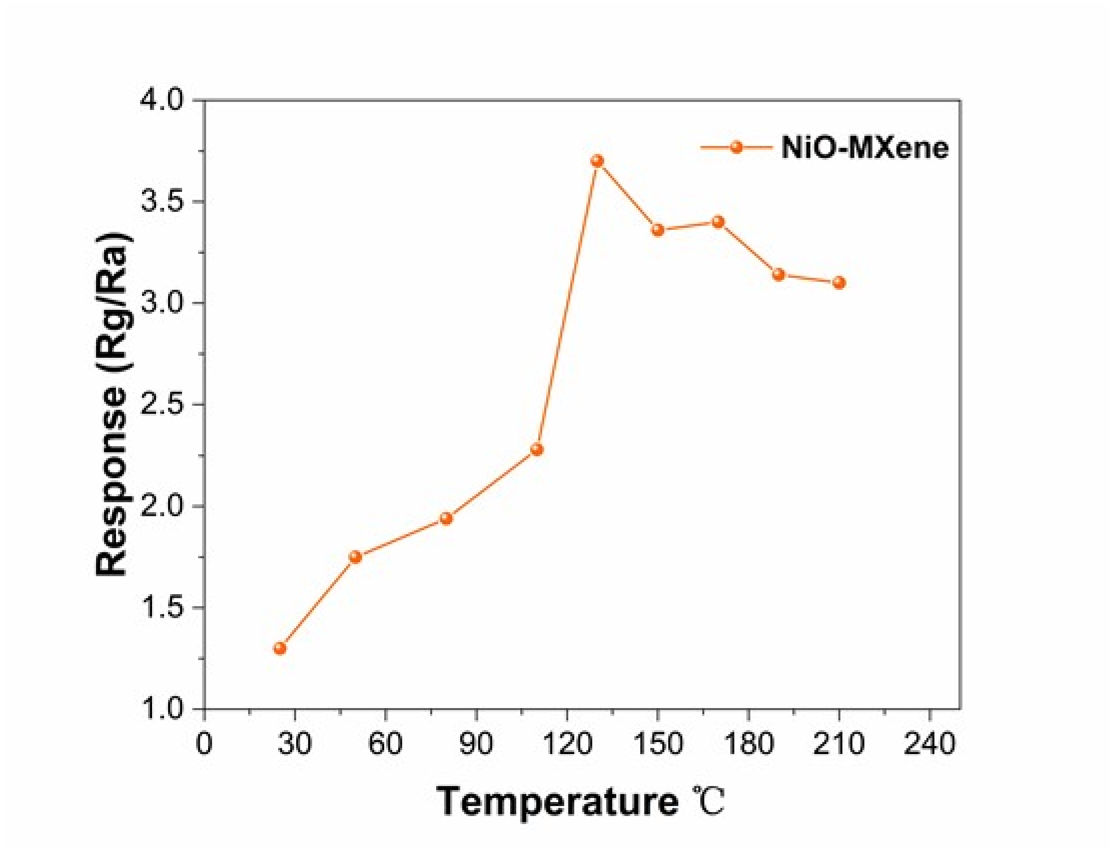



**Fig. S8** The response values of NiO-MXene based sensors to 100 ppm xylene at different operating temperature

**Table S1** Comparison of xylene sensing performance to different gas sensors.

| sample | test gas | Temperature | concn (ppm) | response (%) | Response/ recovery | ref |
|---|---|---|---|---|---|---|
| NiO/$NiCr_2O_4$ | xylene | 225 °C | 100 | 66.2 b | 1217s /591s | [51] |
| Sn-doped NiO | xylene | 225°C | 100 | 20.2b | 298s/223s | [54] |
| W-doped NiO | xylene | 375°C | 200 | 8.62 b | 178s/152s | [53] |
| Au-loaded $MoO_3$ | xylene | 250°C | 5 | 2.5b | 118s/289s | [52] |
| Cr-doped NiO | xylene | 325°C | 50 | 88 b | 144s/50s | [20] |
| NiO/MXene | xylene | 25°C | 500 | 92a | 185s/190s | this work |

**Table S2** Comparison of formaldehyde sensing performance to different gas sensors.

| sample | test gas | Temperature | concn (ppm) | response (%) | Response/ recovery | ref |
|---|---|---|---|---|---|---|
| ZnO-$TiO_2$ | HCHO | 25°C | 20 | 88.9 a | 30s/445s | [55] |
| $In_2O_3$ | HCHO | 420°C | 100 | 1.7 b | 48s/58s | [56] |
| NiO coral like structures | HCHO | 300°C | 190 | 292 a | 24s/42s | [57] |
| Sn-NiO | HCHO | 230°C | 100 | 16.3b | 107s/10s | [58] |
| Pt-loaded NiO | HCHO | 200°C | 1000 | 8.4b | 102s/70s | [59] |
| NiO/MXene | HCHO | 170°C | 100 | 11.4 b | 53s/21s | this work |

**a S= (Rg-Ra) / Ra * 100%**

**b S= (Rg / Ra)**

The Schottky barrier values can be obtained according to the formula of the 2 D thermal electron emission theory, i. e., the relation between current and voltage. The height of the Schottky barrier measured by thermal activation is actually a combination of the I-U method and the activation energy method. The quality factor n, the effective Richard constant $A_{2D}{}^{*}$, and the Schottky barrier height $\Phi_B$ can be determined. If the Schottky barrier is formed on a high-mobility semiconductor, the electron through the Schottky barrier is mainly generated by the hot electron emission effect. The energy level distribution of the thermal electrons satisfies the Fermi-Dirac distribution, so the current I of the barrier and the applied voltage satisfy the following relationship:

$$I = I_0 exp[\frac{q(U - IR)}{nkT} - 1] \text{………(1)}$$

$$I_0 = AA_{2D}^{*}T^2 e^{-q\Phi_B/kT} \text{……………………….(2)}$$

Where A is the contact area of the metal-semiconductor node, $A_{2D}{}^{*}$ is the Richard constant, q is the amount of electron charge, $\Phi_B$ is the Schottky barrier height value, k is the Boltzmann constant, n is the quality factor, and U is the voltage. When q (U-IR) ≥3 kT, there is an approximation:

$$I = I_0 e^{q(U - IR)/nkT} \text{………………………(3)}$$

Regardless of n, R with temperature, n≈1, there is an approximation:

$$I = I_0 e^{qU/kT} = AA_{2D}^{*} e^{q(U - \Phi_B)/kT} \text{……………………….(4)}$$

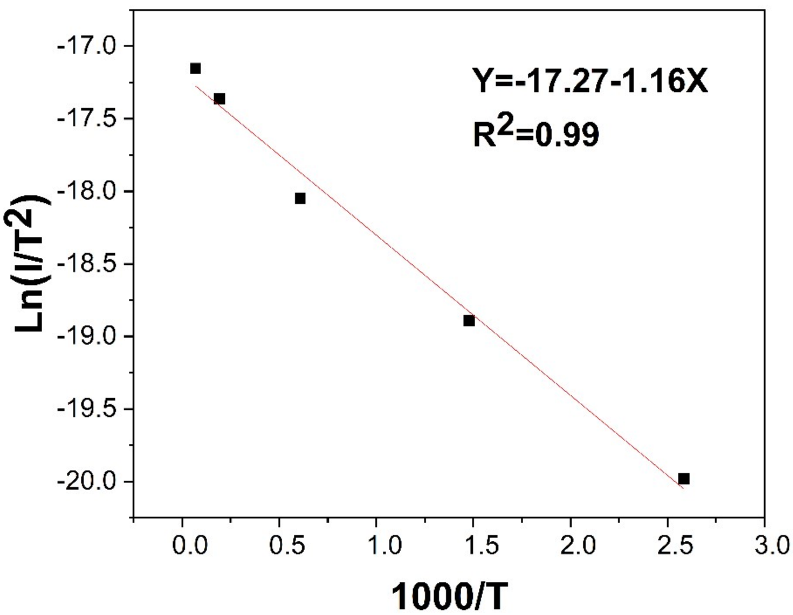
It can be sorted out:

$$In\left(\frac{I}{T^2}\right) = InAA_{2D}^{*} - \frac{q(\Phi_B - U)}{1000k} * \frac{1000}{T} \text{…………………….(5)}$$

Measure the current at different temperatures and make the $In\left(\frac{I}{T^2}\right)-\frac{1000}{T}$ line, and the Schottky barrier height can be determined from the intercept and slope.

| | | | | | |
|---|---|---|---|---|---|
| U(V) | 0.16 | 0.16 | 0.16 | 0.16 | 0.16 |
| I(μA) | 294.14 | 921.48 | 2355.69 | 5189.97 | 7006.79 |
| T(K) | 374.15 | 384.15 | 404.15 | 424.15 | 444.15 |

To obtain the corresponding relationship curve based on the above data:




We can see from the figure that Y=-17.27-1.16X, where $-\frac{q(\Phi_B-U)}{1000k}$ =-1.16 and can obtain $\Phi_B$=0.26V.

**References**

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