



# Transition-metal dichalcogenide NiTe<sub>2</sub>: an ambient-stable material for catalysis and nanoelectronics



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## INTRODUCTION

Following the advent of graphene, the scientific community has widely investigated a large number of layered materials, which have been demonstrated to be effective for a myriad of applications in nanoelectronics, energy storage and sensing [1]. Transition-metal dichalcogenides (TMDs) can also host topologically protected electronic states. For example NiTe<sub>2</sub> has also been predicted to be a type-II Dirac semimetal [2]. Other recent studies have highlighted the capabilities of this material as an electrochemical sensor for glucose detection [3] and for urea conversion [4]. By means of experiments and theory, we assess the surface chemical reactivity and stability of nickel ditelluride NiTe<sub>2</sub>. The Te surface termination forms a TeO<sub>2</sub> skin in an oxygen environment [5]. In ambient atmosphere, passivation is achieved in less than 30 minutes with the TeO<sub>2</sub> skin having a thickness of about 8 Å [5]. Consistently, NiTe<sub>2</sub>-based field effect transistors exhibit superb stability over a timescale as long as one month. Specifically, NiTe<sub>2</sub> has been implemented in a device acting as a millimeter-wave receiver working at 40 GHz, which exhibits both superior performance and environmental stability with respect to graphene and black phosphorus [5].

## RESULTS

### Surface chemical reactivity

XPS core-level Ni-3p and Te-4d spectra collected from as-cleaved NiTe<sub>2</sub> and from the same surface modified by the exposure to 2·10<sup>4</sup> L of CO, H<sub>2</sub>O and O<sub>2</sub>. Strong changes appear only after O<sub>2</sub> exposure. Ni-O component appear in Ni-3p and for the Te-4d oxidation exhibit new components at higher BEs and a further reduction of the intensity of the surface component [6,7].

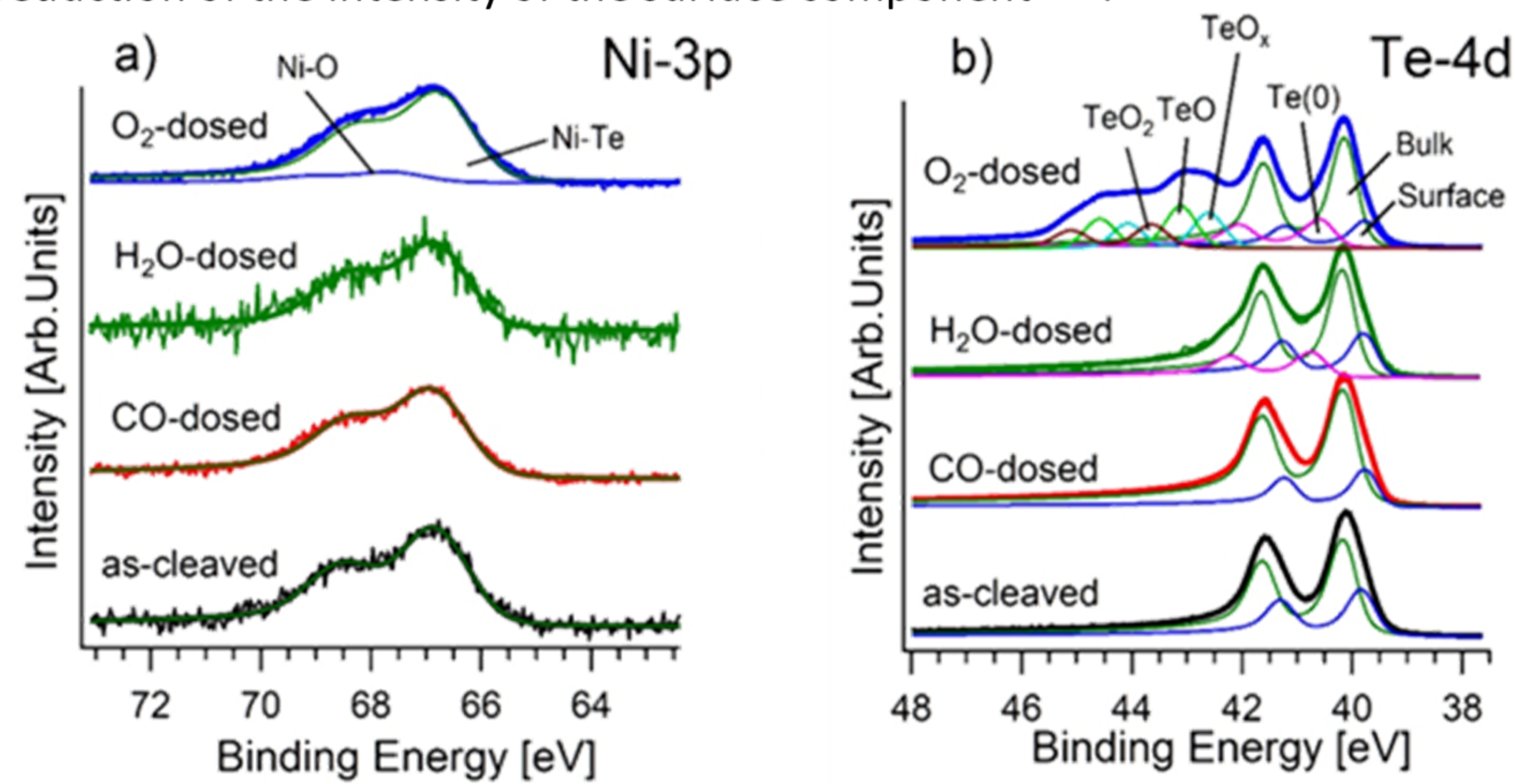


Fig. 1. Core-level Ni-3p (a) and Te-4d (b) spectra collected from as-cleaved NiTe<sub>2</sub> and from the same surface exposed to CO, H<sub>2</sub>O and O<sub>2</sub>. Photon energy is 596 eV and the spectra are normalized to the maximum.

### AFM environmental stability

AFM analyses demonstrate that prolonged exposure to ambient atmosphere does not change the morphology of the flakes (Fig. 2a-d), as confirmed by the height profile along a specific direction remaining constant with time (Fig. 2e).

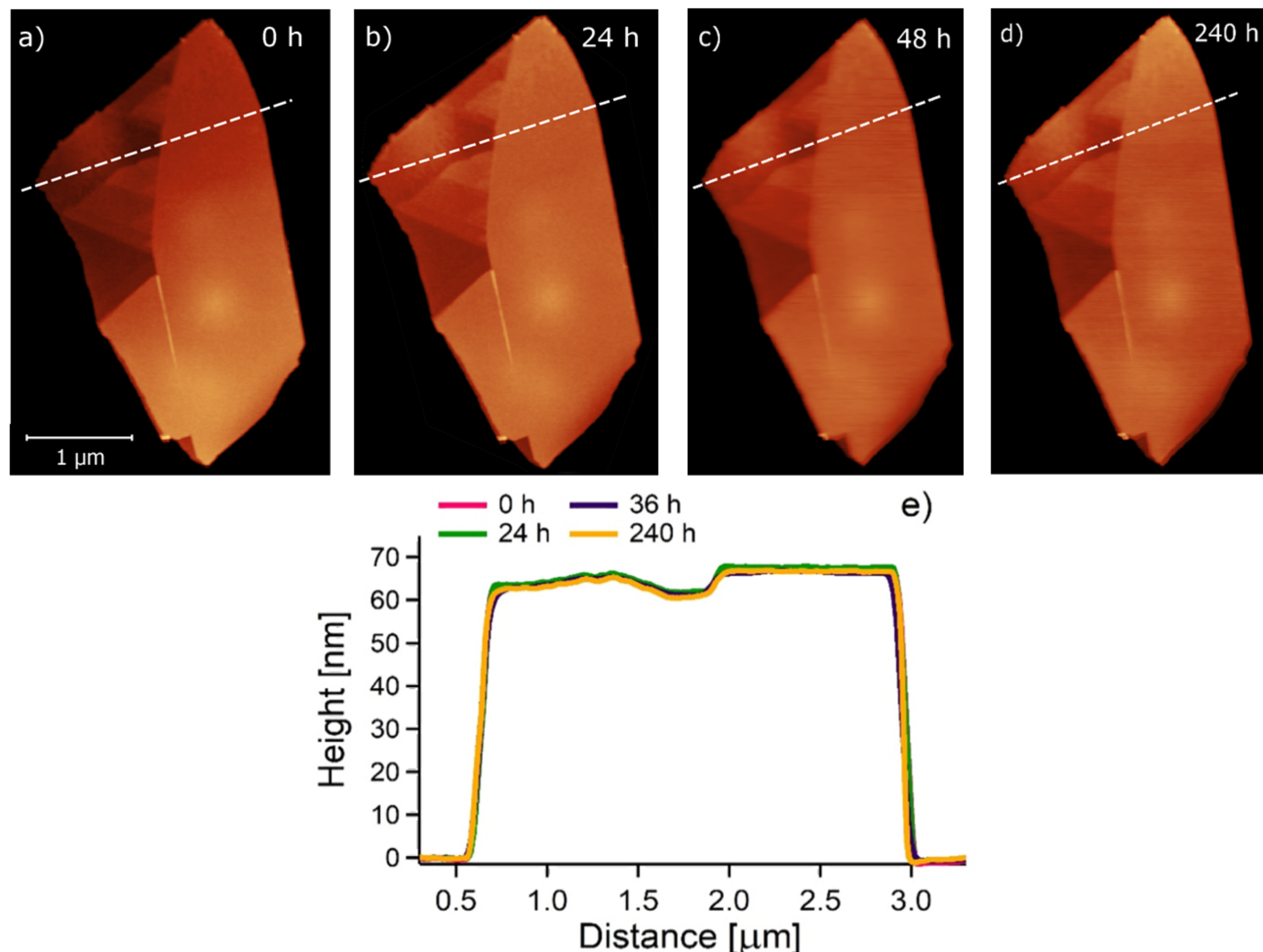


Fig. 2. Time evolution of AFM images of a ~60 nm thick flake of NiTe<sub>2</sub>. Panel (a) shows the flake immediately after exfoliation, while panels (b)-(d) show the same flake after 24, 48 and 240 hours in air, respectively. The dotted white lines indicate the path of the height profile shown in panel (e).

### Aging study in ambient atmosphere

In ambient atmosphere, passivation is achieved in less than 30 minutes with the TeO<sub>2</sub> skin having a thickness of about 8 Å. A prolonged exposure time (up to 41 hours) does not induce further oxidation of the NiTe<sub>2</sub> surface, while TeO and TeO<sub>x</sub> are both converted to TeO<sub>2</sub>. The NiO component reaches a maximum of 58% of the Ni-3p total spectral area after 30 minutes, and no further increase after a longer storage time in ambient air was observed.

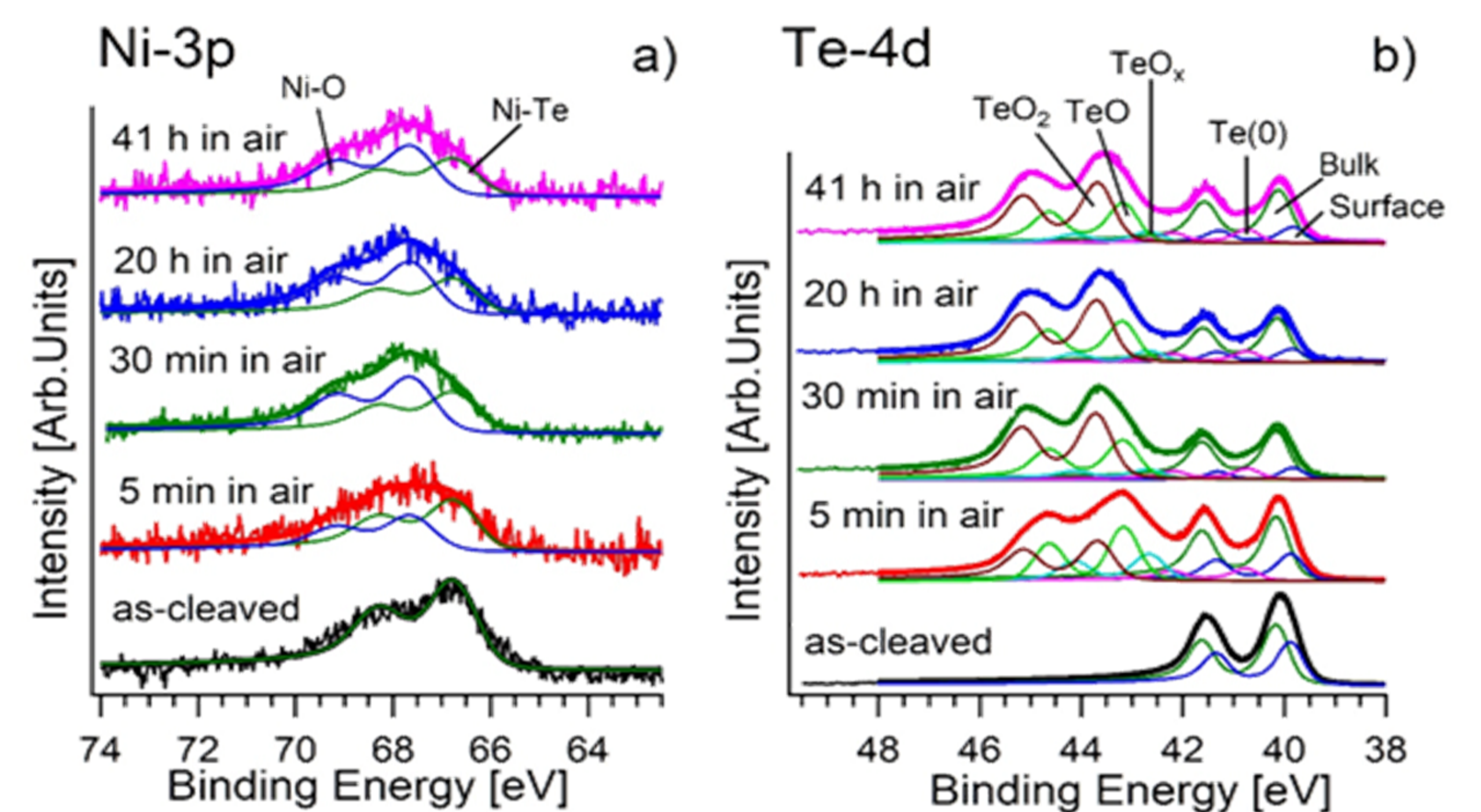


Figure 3. Core-level Ni-3p (a) and Te-4d (b) spectra collected from NiTe<sub>2</sub> exposed to air for 5 min, 30 min, 20 h and 41 h. Photon energy is 596 eV and the spectra are normalized to the maximum.

### Device implementation

NiTe<sub>2</sub>-based field effect transistors exhibit superb stability over a timescale as long as one month.

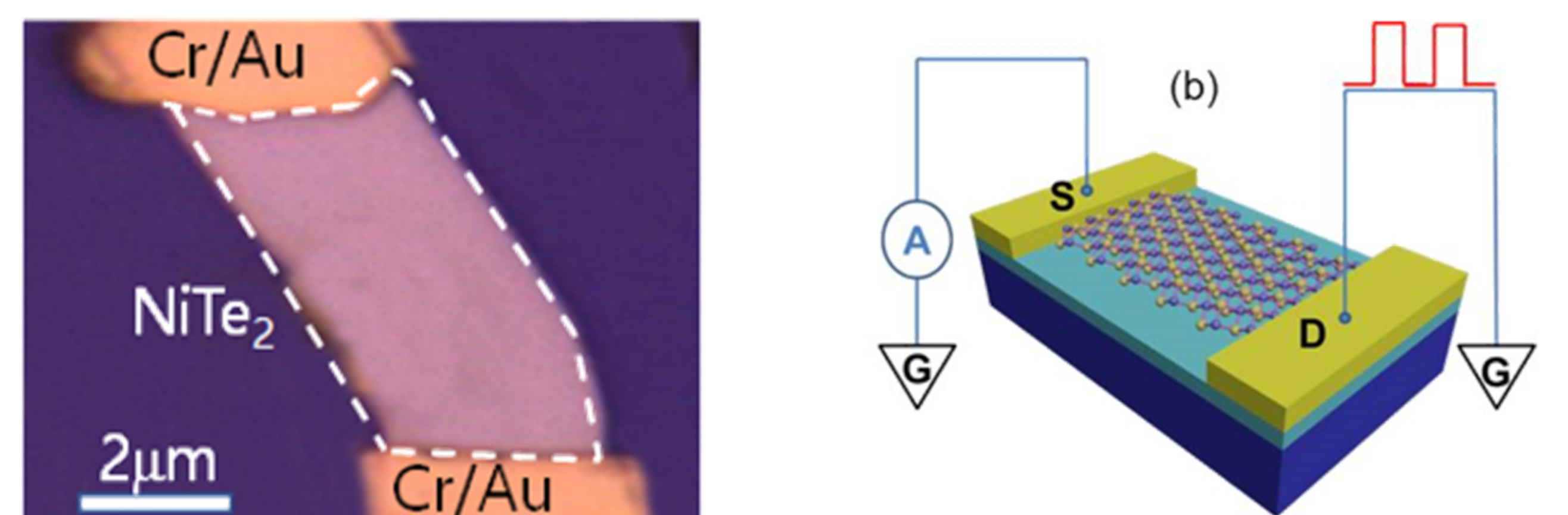


Fig. 4. (a) Optical microscopy of NiTe<sub>2</sub>-based FET obtained from mechanically exfoliated bulk single crystal. (b) Schematic diagram of the nanodevice with a NiTe<sub>2</sub>-based active channel.

Tab 1. Comparison of the performance of receivers based on graphene, black phosphorus and NiTe<sub>2</sub> at 40 GHz carrier frequency.

	graphene	black phosphorus	NiTe <sub>2</sub>
<b>Responsivity (A/W)</b>	1.50±0.01	0.74±0.01	5.18±0.01

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## CONCLUSIONS

Bulk NiTe<sub>2</sub> is an ambient-stable material with diverse applications, ranging from catalysis to nanoelectronics. A passivating TeO<sub>2</sub> overlayer is formed after exposure to ambient atmosphere for less than 30 minutes. The passivated surface is stable in air over a timescale of several weeks. The NiTe<sub>2</sub> surface does not show any reactivity toward H<sub>2</sub>O and CO, enabling the possibility to fabricate CO-tolerant electrodes. Furthermore, devices with active NiTe<sub>2</sub> channels exhibit high stability in air even without encapsulation. Finally, we tested the suitability of NiTe<sub>2</sub> for high-frequency electronics. The signal exhibits especially good repeatability without decay even after a one-month exposure to the ambient environment.