Electronic Supplementary Material (ESI) for Analytical Methods.


**Supplementary Information**

# Highly sensitive and selective detection of 2,4,6-trinitrotoluene (TNT) explosive using a peptide functionalized silicon nanowire sensor

Xingqi Liu[a, b], Hongpeng Zhang[a], Zhiping Huang[a], Zhenxing Cheng[a]*, and Tie Li[b]*

[a]Department of Chemical Defense, Institute of NBC Defense, PLA Army, Beijing 102205, China.

[b]Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, Shanghai 200050, China.

*Corresponding authors: Zhenxing Cheng, Email: chengzx2018@sina.com; Tie Li, Email: tli@mail.sim.ac.cn

## 1. Fabrication of SiNW devices

The fabrication for SiNW devices starts from a 4-inch (111) silicon-on-insulator (SOI) wafer. Firstly, 100 nm silicon nitride ($Si_3N_4$) layer was deposited on the top of SOI wafer using the LPCVD process. Then, corrosion windows were patterned on the $Si_3N_4$ layer and the silicon underneath is moved by reaction ion etching. After anisotropic etching methods in 40 wt% KOH solution, silicon nano-walls were generated between the adjacent etched cavities in a controllable size-reduction process, and inverted-triangle silicon nanowires arrays were generated on the top center of walls arrays by self-limiting oxidation. Then again, the source and drain location were heavily doped by ion implantation process and covered with a gold layer. Finally, SiNW array devices were generated after removal of oxidization layer.

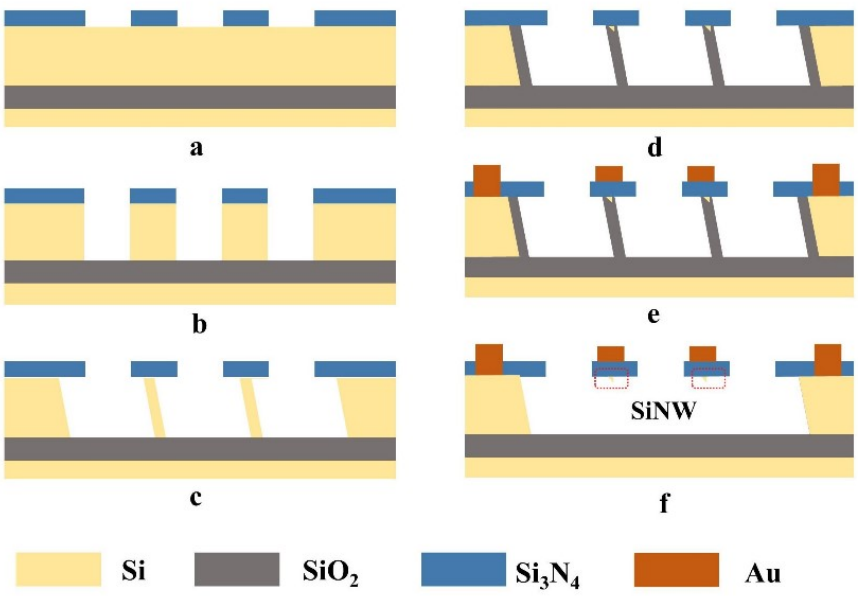


Fig. S1 Fabrication of SiNW devices on 4-inch (111) SOI wafer.

## 2. Chromatogram and MS Spectrum of anti-TNT peptide

To characterize the peptide aptamer samples obtained by synthesis, the peptide samples were purified by running through a silica gel chromatography column and the purified compound was subjected to mass spectrum (MS) analysis.

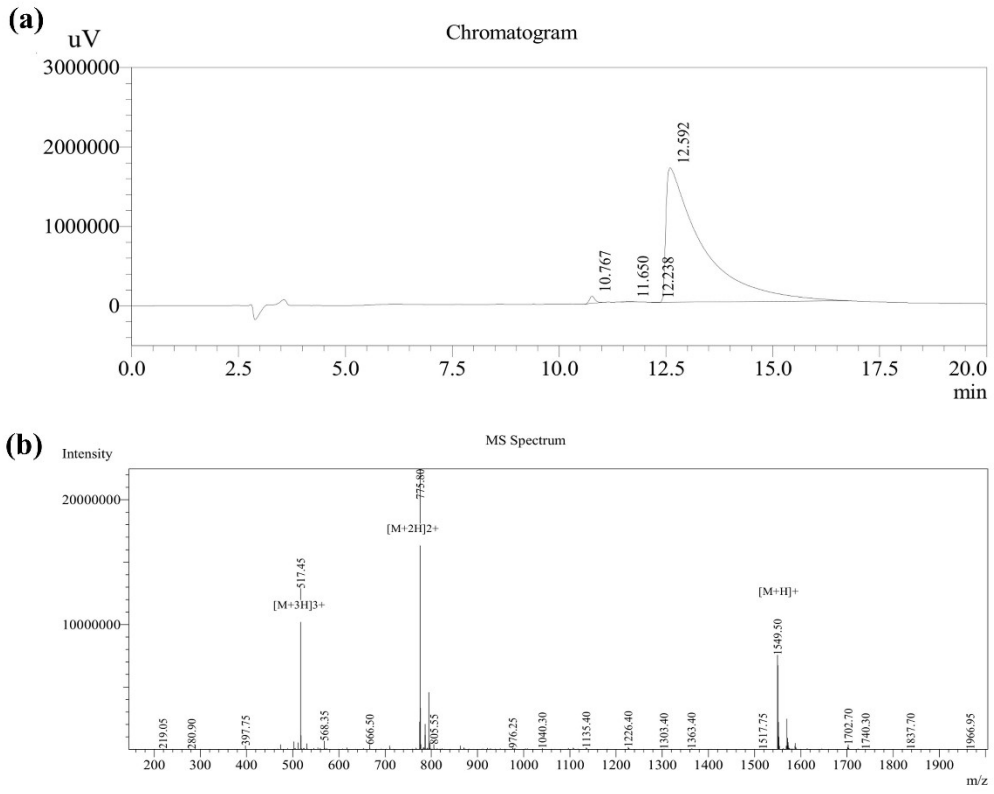


Fig. S2. Chromatogram and MS Spectrum of anti-TNT peptide.

## 3. Sensing apparatus and parameters

The SiNW chip is connected to a 1.5 × 1.5 $cm^2$ PCB (printed circuit board) as a sensor unit by gold ball wire bonding. During TNT sample testing process, SiNW sensors were deployed at a homemade testing chamber. Electrical connections within the testing chamber were made with a zero-insertion force (ZIF) socket and a simple printed circuit board for easy loading and unloading of SiNW sensors. A Keithley 4200 semiconductor were connected to the circuit board of the sample chamber to record current signals.

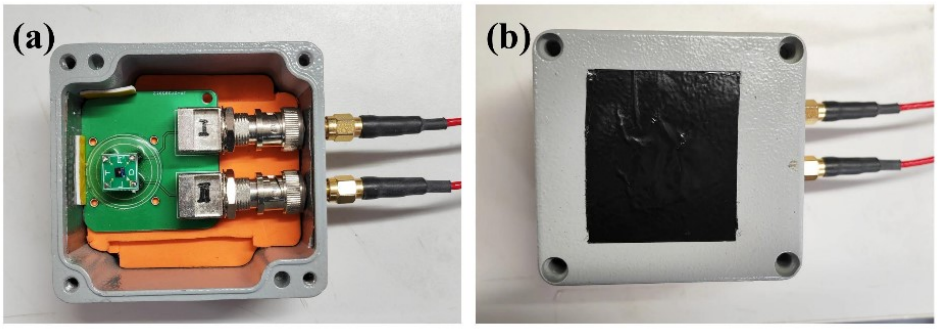


Fig. S3. The photos of testing chamber of SiNW senor.

**4. Detection of TNT Vapor**

Meanwhile, there has been considerable interest in the detection of nitro aromatic vapors. After 24 hours at room temperature, the saturated vapor of TNT was produced in a sealed Teflon air sampling bag and further diluted to certain concentrations.

As shown in the figure, the sensor current drops immediately when exposed to TNT vapor at the sub-ppb level in air. Then, after the sealed chamber is opened to fresh ambient air, the device current returns to near baseline. This is a typical adsorption-desorption process for gas sensors and means that our sensor can detect TNT in a gas-phase environment.

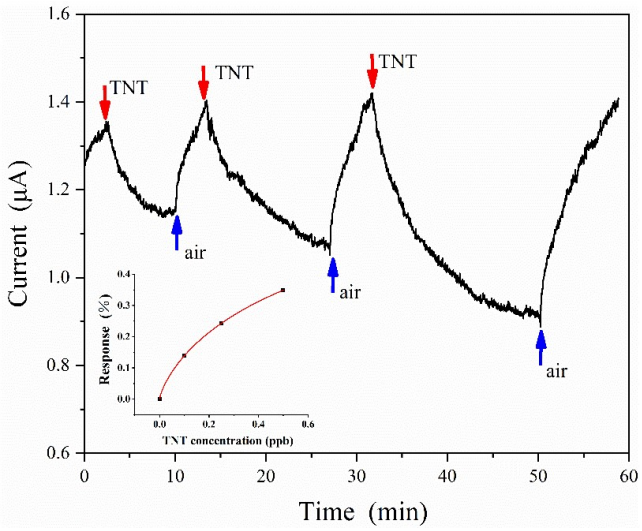


Fig. S4. Real-time current response to TNT vapor at the sub-ppb level in air.

**5. Calculation of the Debye length**

According to Debye screening, the charge change in biometric recognition cannot be detected over a certain distance. This screening length is quantified by the Debye length ($\lambda_D$), which is defined as:

$$\lambda_D = \sqrt{\frac{\varepsilon k_B T}{q^2 c}}$$

where $k_B$ is Boltzmann's constant, T is the temperature, q is the electron charge, c is the ionic strength of the electrolyte, and ε is the dielectric permittivity of the medium. At the same dielectric and absolute temperature, the lower concentration of PBS buffer solution corresponds to the larger $\lambda_D$. According to equation 2, the Debye lengths of different concentrations of PBS buffer solutions over a range from 0.1 × PBS to 0.0001 × PBS can be calculated, and the results are shown in the table below.

Table S1: Debye length of different concentrations of PBS buffer solution

| PBS | $\lambda_D$（nm） | ionic strength (mM) |
|---|---|---|
| ×0.1 | 2.3 | 15 |
| ×0.01 | 7.3 | 1.5 |
| ×0.001 | 23.2 | 0.15 |
| ×0.0001 | 75 | 0.015 |

**6. Sensor calibration.**

The biochemical detection mechanism of silicon nanowire sensors is similar to the photoresponse mechanism in that they both affect the silicon nanowire channel of the inner carrier concentration to change the device current. This special characteristic can be used to calibrate the sensors, without any damage or harm to the sensor.

A typical photoresponse and target-response result of SiNW array sensor is shown in Fig. S2a, the trends of the sensor signals are clearly very similar and both fit Langmuir-Freundlich adsorption model. Fig. S6b shows the linear correlation relationship in logarithmic coordinates. Based on the relationship between light response and target response, we calibrated the response of the sensor to TNT, and the results are shown in Fig. It is clear that sensor calibration methods can effectively improve the consistency of response to TNT.

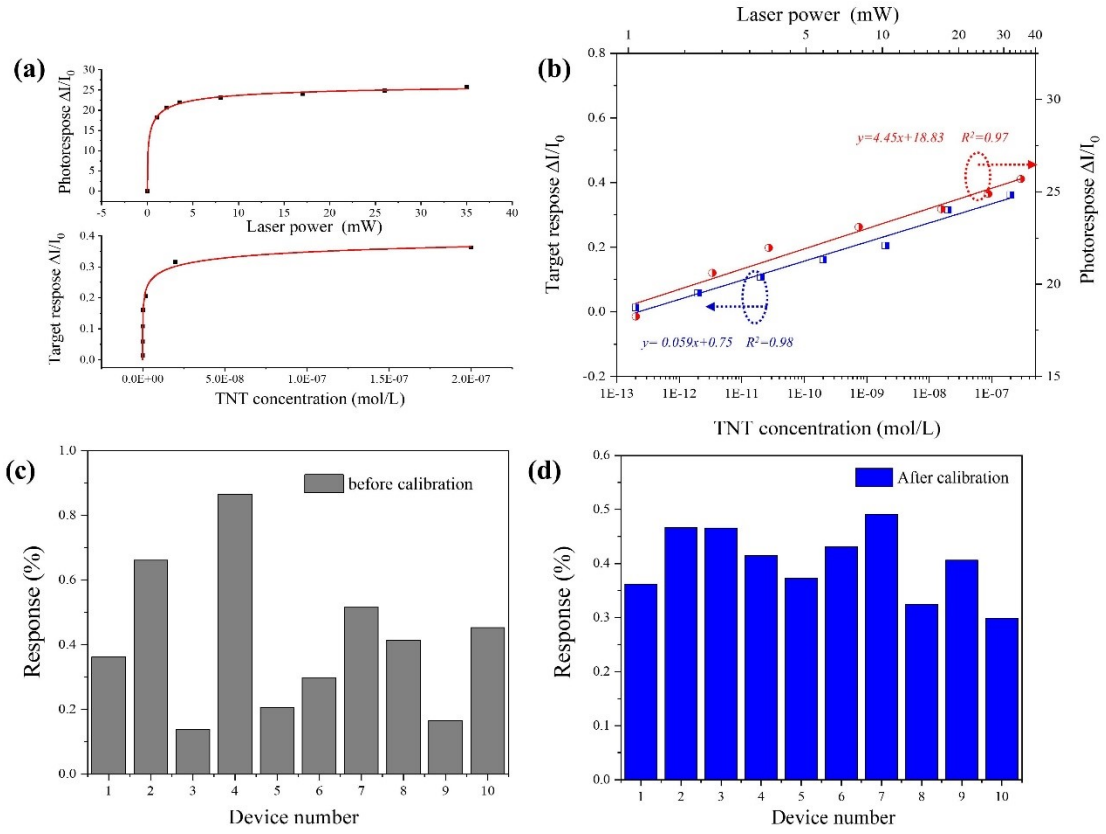

Fig. S6. Sensor calibration using light simulation. (a) a typical photoresponse and target-response result of SiNW array sensor (b) fitted linear relationship in logarithmic coordinates (c) Distribution of the response to TNT without calibration (d) Distribution of the response to TNT with calibration.