Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supporting Information for

Iron Oxide Nanowires Based Filter for Inactivation of Airborne Bacteria

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Simulation

The temperature gradient around the IO NWs filters was simulated using COMSOL Multiphysics®. The model was integrated by three parts (Equation 1-3).[1] The detailed description of the equations and parameters is shown in the Supporting Information.

$$\nabla(\sigma \times \nabla V) = 0 \tag{1}$$

$$\rho \times u\nabla u - \mu\Delta u + \nabla p = 0 \tag{2}$$

$$k\nabla^2 T + C_p \times \rho \times u \times \nabla T = \sigma \times |\nabla V^2| \tag{3}$$

The module simulated an opening of iron mesh (200 μm × 200 μm), where the iron wire has a diameter of 200 μm and is covered with a layer of iron oxide (thickness = 0.5 μm). The size of the air flow channel is 600 μm×600 μm×1400 μm. The meshes were made up of 39827 meshes.

Equation (1) is the solution for the electrical potential distribution in the cell, where V is the voltage and σ is the electrical conductivity of the media. Equation (2) is the classical incompressible Navier-Stokes equation, where ρ is density of air, u is velocity of air and p is the pressure. Equation (3) is the conductive and convective heat transfer equation with Joule heat as source, where k is the conductive heat transfer coefficient, T is the temperature, C_p is the heat capacity of air and $\sigma \times |\nabla V^2|$ is Joule heating term.

The electrochemical field near the IO NWs was also simulated using the COMSOL Multiphysics® software package. The static electricity model was selected. A cubic zone with size of 26 μm × 26 μm× 26 μm, and a nanowire with size of 0.06

μm (radius) × 13 μm (length) was simulated. The material of the cubic zone is air and the material of the nanowire is Fe_2O_3. The voltage applied on the nanowire was 4.5 V.

Supplementary Tables

Table S1. Calculation of capture efficiency of the two types of filters (voltage = 0 V).

Filter	Treatment time (s)	$N_{captured}$ (10^9 CFU)	$N_{escaped}$ (10^9 CFU)	$r_{captured}$ (%)
IO NWs	10	3.6	6.8	52.9
	20	4.6	8.9	51.7
	30	6.4	12.3	52.0
Pristine Iron mesh	10	2.3	7.1	32.4
	20	3.1	10.2	30.4
	30	5.0	13.7	36.5

Table S2. The number of bacteria escaped from the IO NWs filter

Voltage (V)	Treatment time (s)	$N_{escaped}$ (10^9 CFU)	Percent deviation (%, compared to 0 V)
1.5	10	7.1	4.4
	20	8.7	-2.2
	30	12.7	3.3
3	10	6.9	1.5
	20	9.3	4.5
	30	11.3	-8.1
4.5	10	6.2	-8.8
	20	9.6	6.7
	30	12.8	4.1

Supplementary Figures

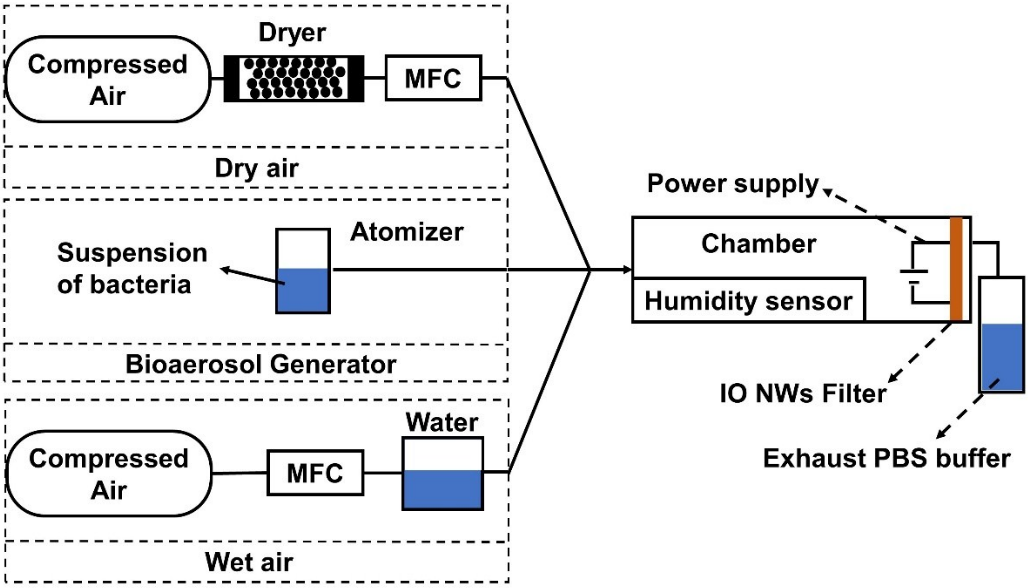

Fig. S1. Schematic illustration of the experimental set-up for the generation and inactivation of S. epidermidis bioaerosols. The applicability of resuspending the filter into PBS buffer to measure the bacteria concentration was verified by a controlled experiment. Firstly, we measured the bacteria amount in the exhaust PBS buffer ($N_{buffer-1}$) when no IO NWs filter was employed, the operation time was set to be 30 s. Then, we measured the bacteria concentration in the exhaust PBS buffer ($N_{buffer-2}$) and that on the IO NWs filter (N_{filter}, by resuspending the filter into PBS) when one filter was placed in the front of exhaust buffer. The operation time was also 30 s (no voltage was applied). It was found that $N_{buffer-1} \approx N_{buffer-2} + N_{filter}$. As a result, the above measurement method for estimating the bacteria amount on the filter by resuspending into PBS was applicable. Meanwhile, the IO NWs filter is proven to be of no disinfection ability when no voltage is applied in this way.

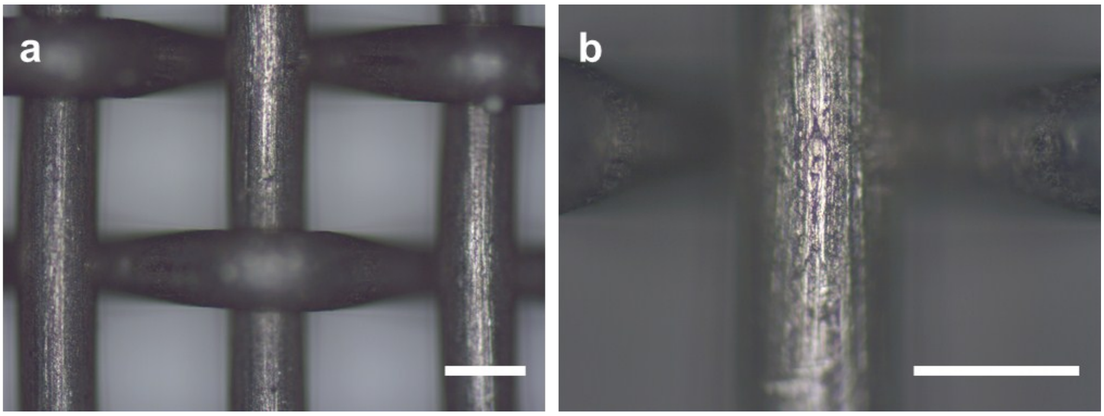

Fig. S2. Optical microscopy images of pristine iron mesh under (a) low and (b) high magnification. Scale bars represent 200 μm.

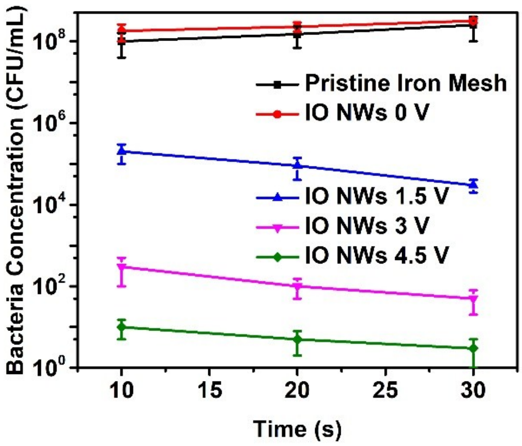

Fig. S3. Measured bacteria concentrations by resuspending the filter into the PBS solution. The corresponded bacteria amount can be obtained by multiplying the concentration by the volume of PBS solution (20 mL).

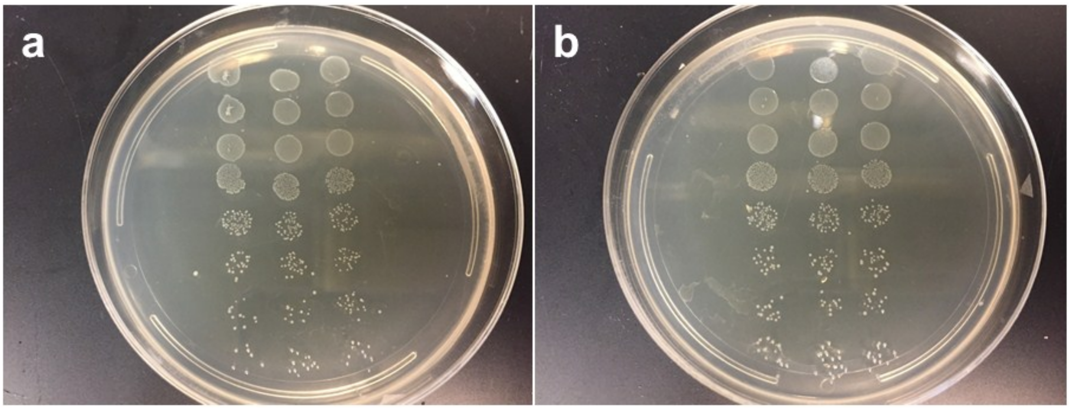

Fig. S4. Effect of DMSO on the bacteria. (a) is the fresh bactera, (b) is the bacteria mixed with PBS solution of DMSO (100 mM) for 5 min. No significant difference between the two samples was observed, indicating that DMSO is not lethal to the bacteria.

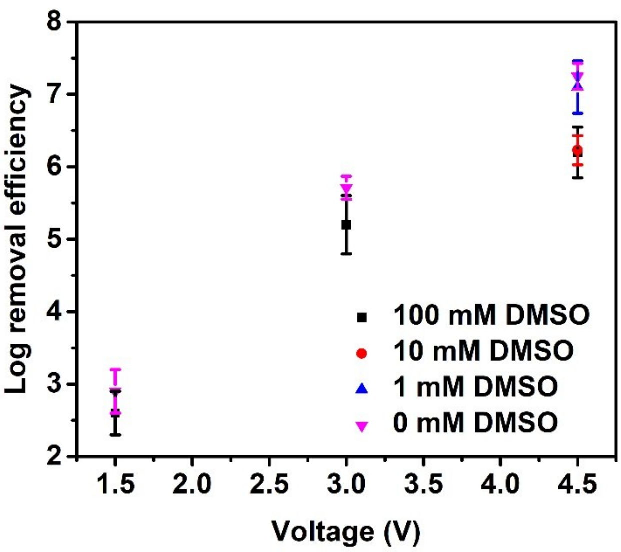

Fig. S5. The effect of DMSO on the inactivation performance. Under voltages of 1.5 V and 3.0 V, only 100 mM of DMSO was used because this amount is enough to quench ROS as verified at 4.5 V.

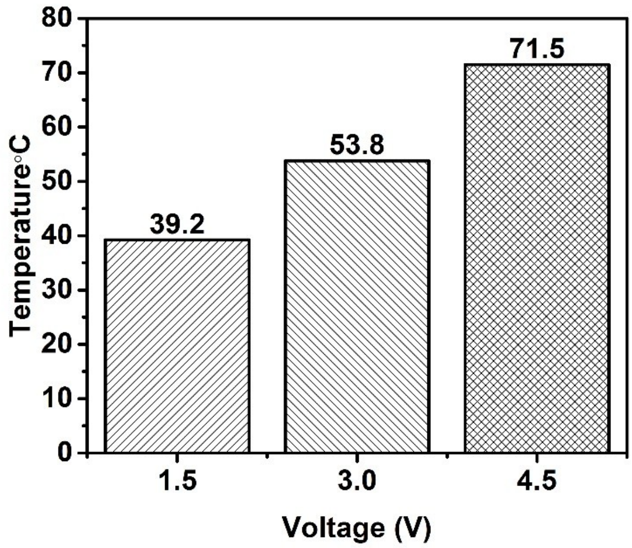

Fig. S6. Bulk surface temperatures of the IO NWs filter varied with different applied voltages (air flow velocity = 0 m/s).

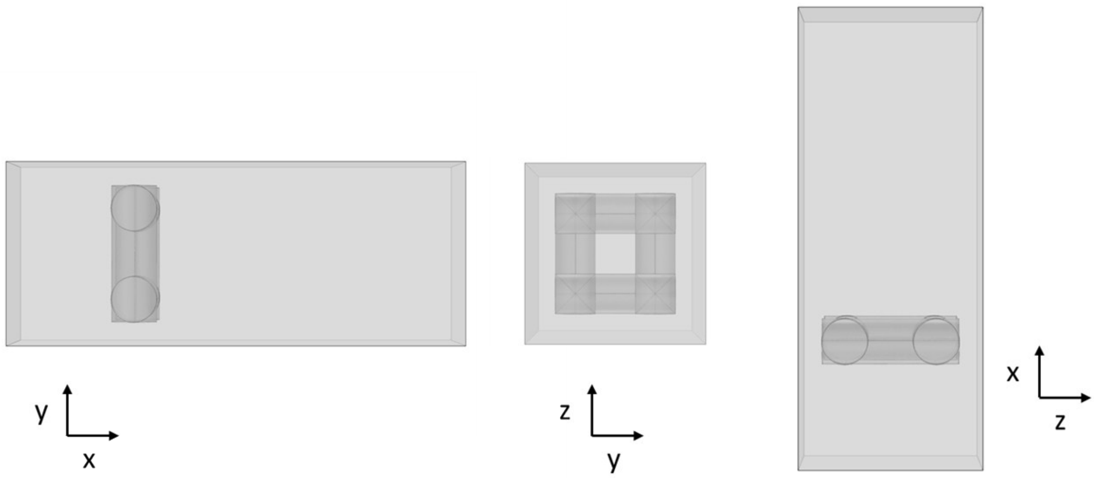

Fig. S7. Three-view drawing of the simulation unit for temperature gradient.

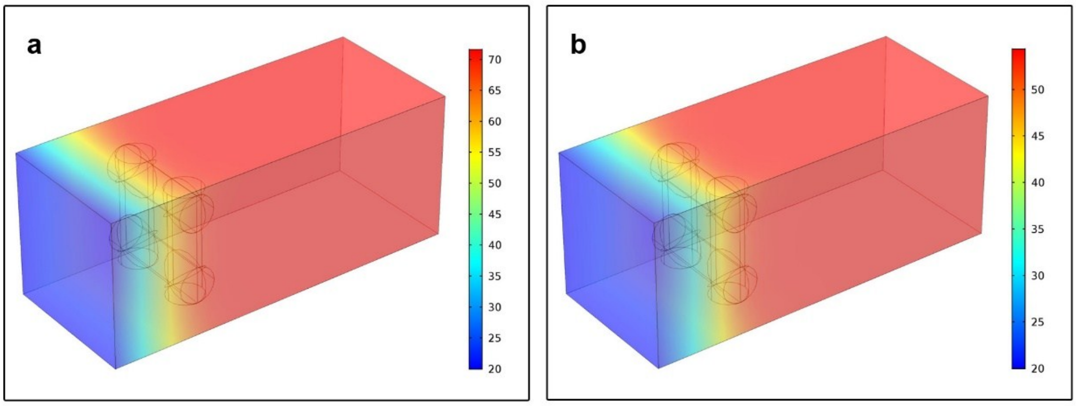

Fig. S8. Effect of air flow rate on the temperature gradient near the IO NWs filter. (a) flow rate = 0.5 m/s, and (b) flow rate = 5 m/s.

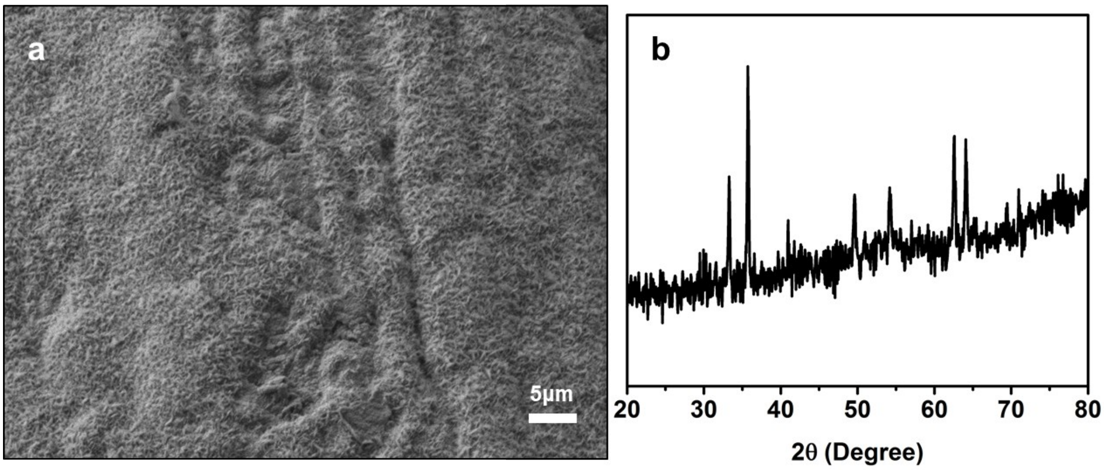

Fig. S9. IO nanoparticles on iron mesh. (a) SEM image and (b) XRD pattern. IO nanoparticles on iron mesh were obtained by heating the mesh in the air to 700 °C from room temperature (5 °C/min). Once the temperature reached 700 °C, the mesh was taken out from the furnance.

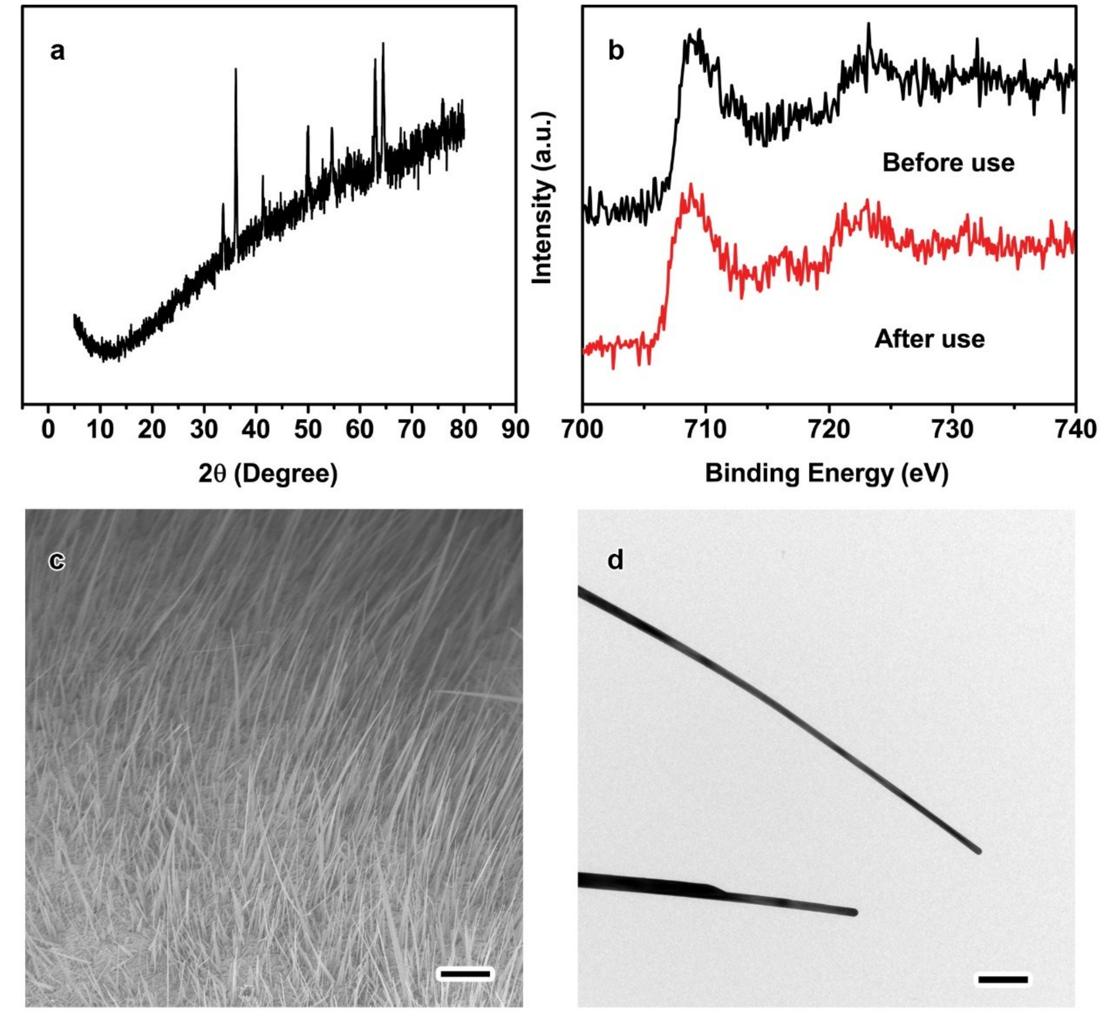

Fig. S10. (a) XRD pattern, (b) XPS spectra for Fe 2p, (c) SEM image, and (d) TEM image of the IO NWs after five cycles of 1 h operation. Scale bars in (c) and (d) represent 5 μm and 500 nm, respectively.

Reference

1. A. V. Dudchenko, C. Chen, A. Cardenas, J. Rolf and D. Jassby, Frequency-dependent stability of CNT Joule heaters in ionizable media and desalination processes, *Nature Nanotechnol.*, 2017, **12**, 557-563.