Supplementary Information

Self-Powered Monitoring of Ammonia Using an MXene/TiO_2/Cellulose Nanofiber Heterojunction-Based Sensor Driven by an Electrospun Triboelectric Nanogenerator

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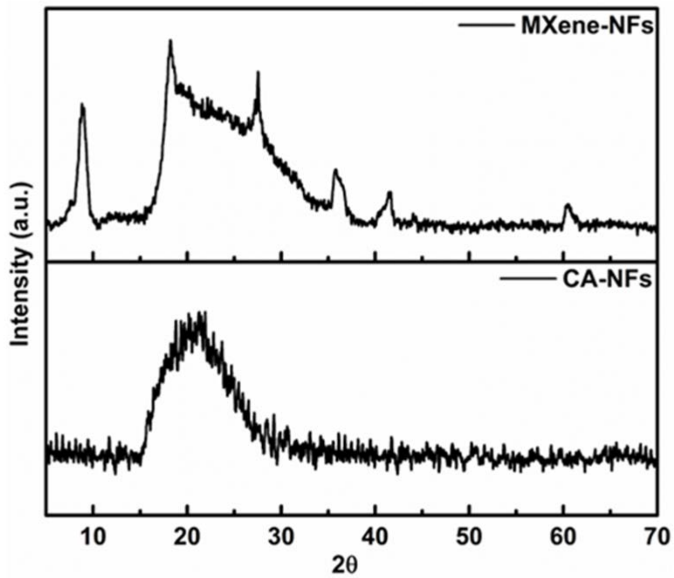


Figure S1. XRD spectra of (a) MXene-NFs and CA-NFs

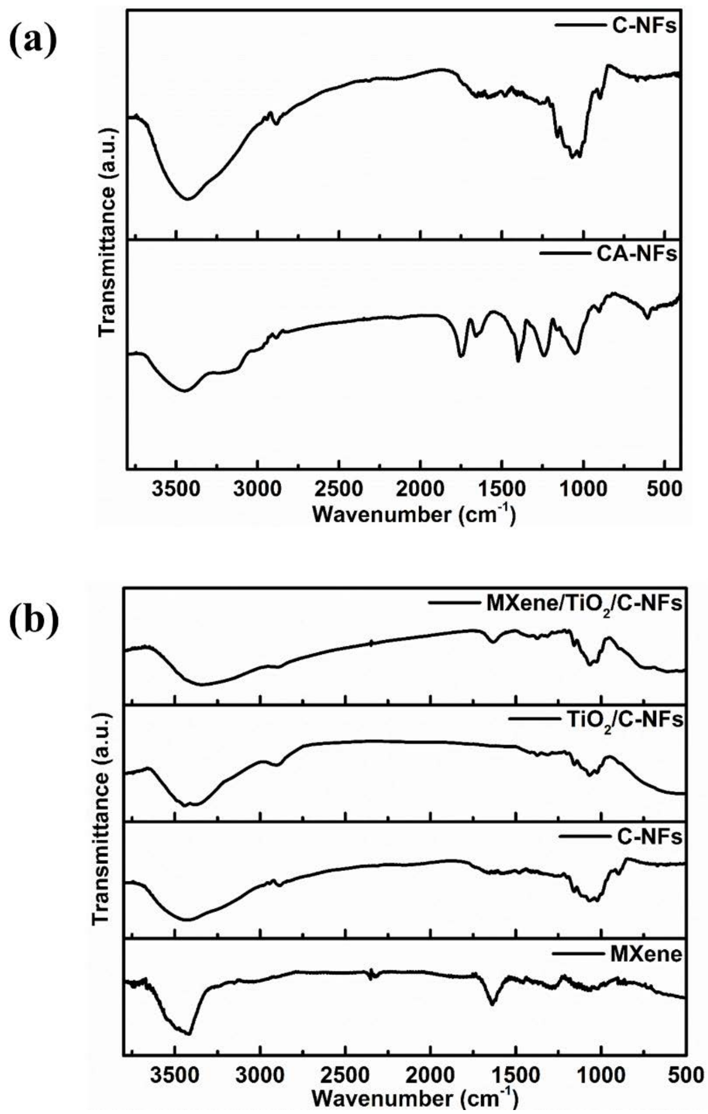


Figure S2. FTIR spectra of (a) CA-NFs and C-NFs and (b) MXene, C-NFs, TiO_2/C-NFs and MXene/TiO_2/C-NFs heterojunctions based sample

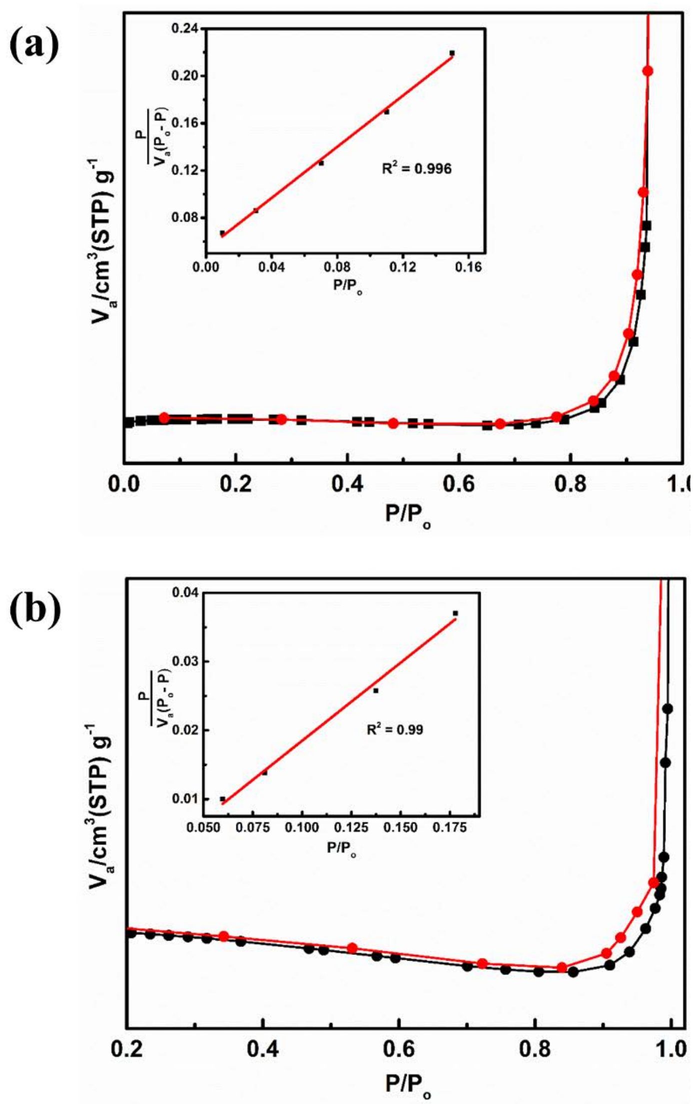


Figure S3. BET studies of (a) MXene and (b) MXene/TiO_2/C-NFs heterojunctions based sample

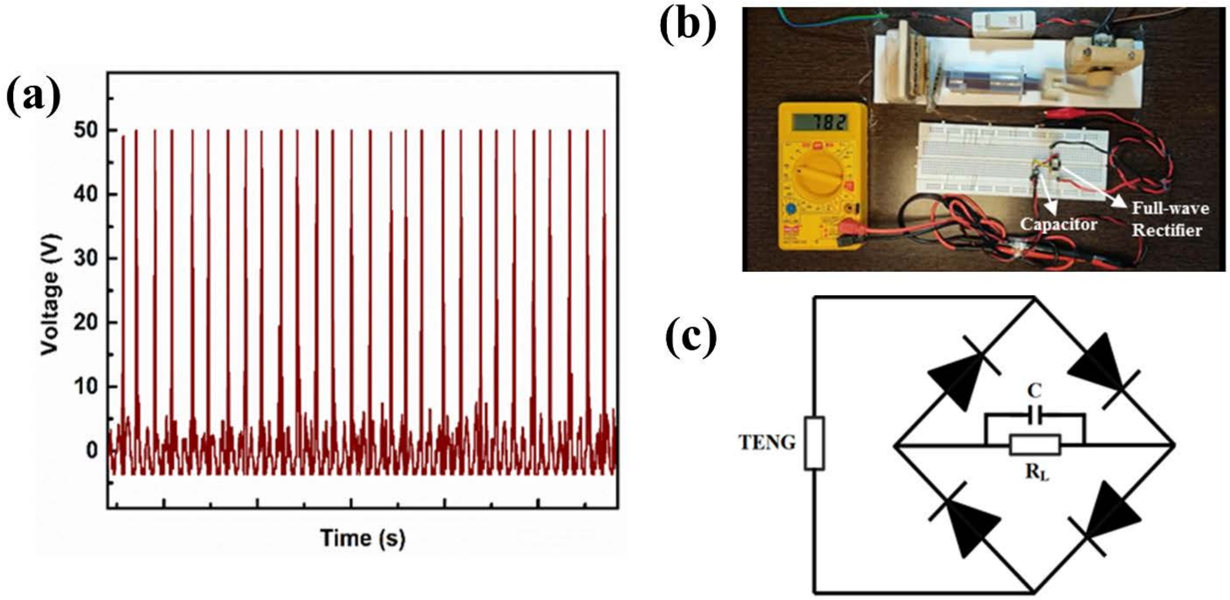
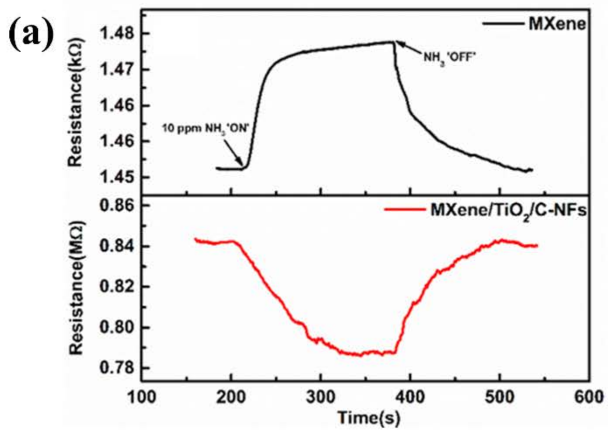
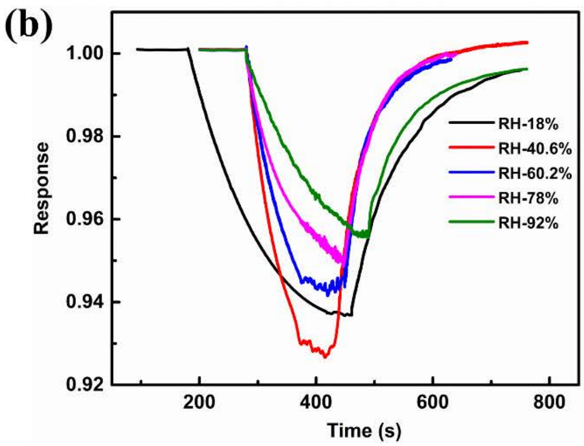


Figure S4. (a) Output DC voltage of MXene/CA-NFs combination based TENG, (b) Photograph of capacitor charging, (c) Equivalent circuit used to charge 4.7 μF capacitor.





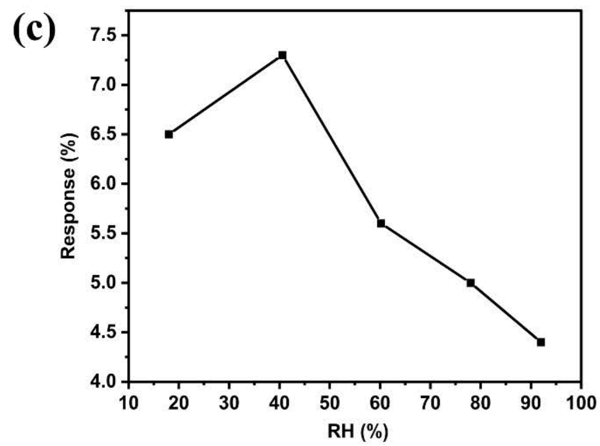


Figure S5. (a) Resistance-time graph of MXene and MXene/TiO_2/C-NFs heterojunctions based sensor for 10 ppm NH_3 at room temperature, (b) Response curves of MXene/TiO_2/C-NFs heterojunctions based sensor and (c) Response (%) variation for different relative humidity.

DFT calculations:

Structure optimization and band gap calculations of MXene and TiO_2 were carried out by the Vienna ab initio simulation package (VASP) code using MedeA as graphical user interface. Generalized gradient approximation (GGA) with the Perdue Burke–Ernzerhof (PBE) was employed for the exchange–correlation function. Using the conjugate gradient algorithm, the positions of atoms were fully relaxed and total energies were well converged to 10^{-6} eV. The cut off energy of 520 and 400 eV for MXene and TiO_2, respectively, were set for plane wave basis set. The Brillouin zone integration was sampled by Monkhorst–Pack k-point mesh for geometry optimizations of 5 ×5 × 1 grid of MXene and 6 × 6 × 6 grid of TiO_2. Finally, the band structures of fully relaxed unit cells of MXene and TiO_2 were carried out with a finer mesh of 10 × 10 × 1 and 10 × 10 × 10 k-points, respectively. A vacuum space of 15 A˚ was added along the c-axis direction of MXene layer to avoid inter layer interaction.

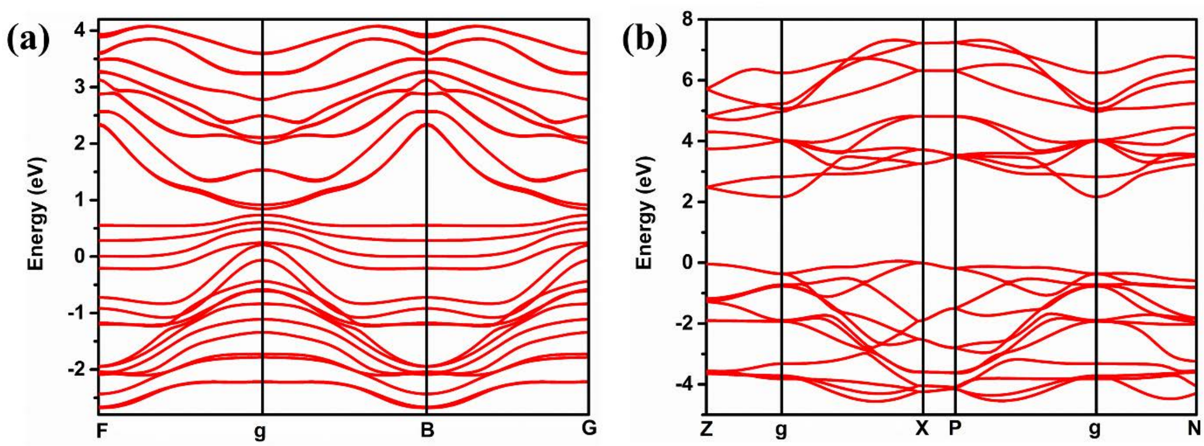


Figure S6. (a) Band Structure of (a) MXene and (b) TiO_2 unit cell

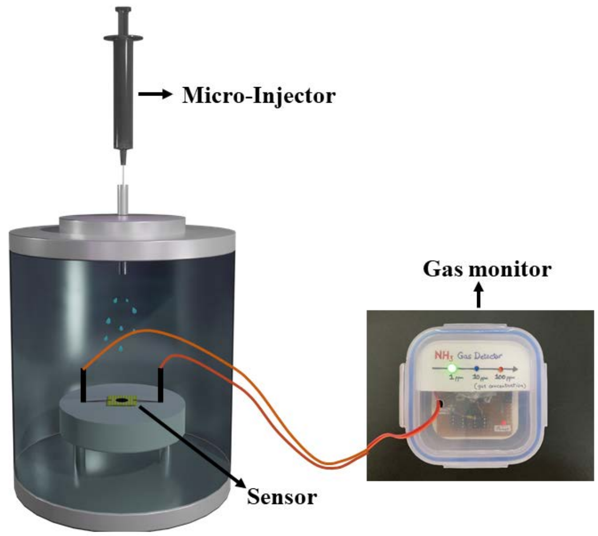


Figure S7. A gas monitoring device

Video S1: The working of home-made tapping device; charging of capacitor and powering of LEDs using TENG.

Video S2: The working of NH_3 monitoring device; NH_3 concentration at 1 ppm, 10 ppm and 100 ppm can lighten three different LEDs.

Video S3: The monitoring device embedded in shoe insoles is directly driven by TENG.