Supporting information

Bandgap Engineering in Efficient Solar-driven Interfacial Evaporation System

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1 Evaporation system and outdoor desalination system

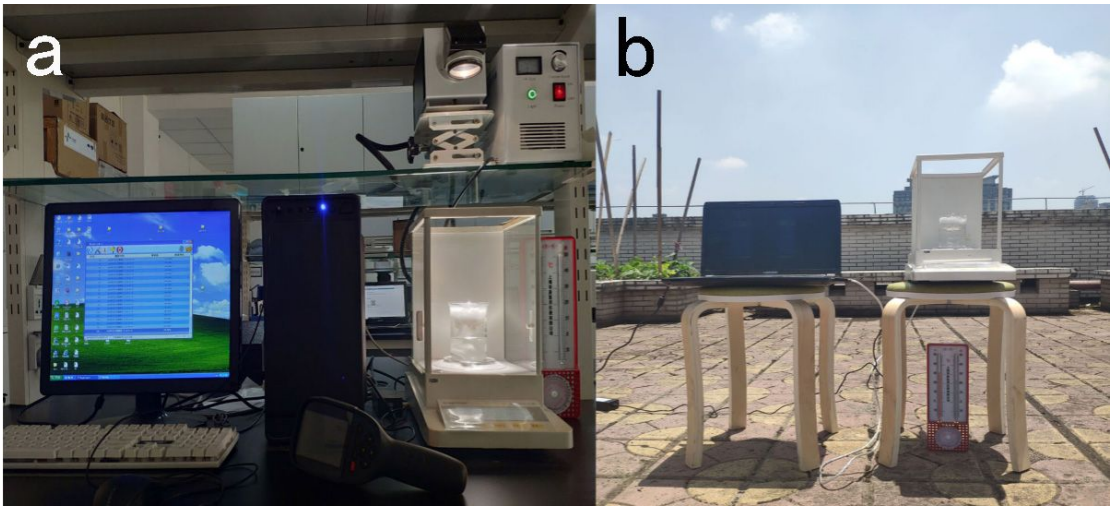

Figure S1. (a) Evaporation system and **(b)** Outdoor desalination system. The systems are mainly consisted by balance with accuracy of 0.1 mg, computer for recording weight at each minute, 200 ml beaker with Polyethylene foam thermal insulators and psychrometer. Simulative light source is equipped to simulate sunlight (AM1.5) in evaporation system.

2 Evidence of nitrogen doping in N, Ti^{3+}-TiO_2.

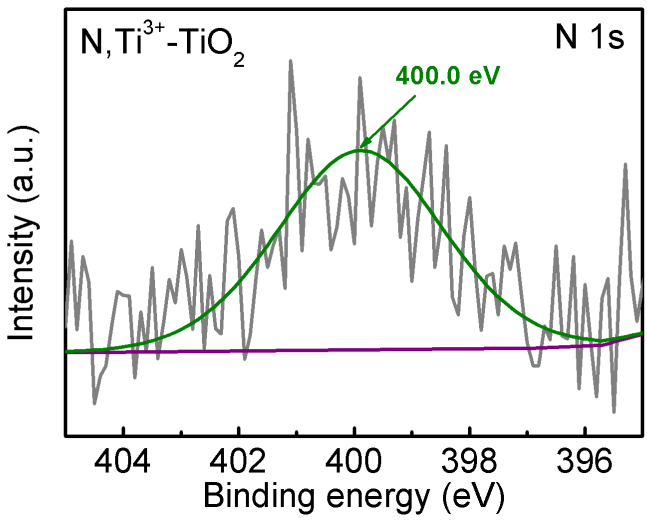

Figure S2. N1s spectrum of N, Ti^{3+}-TiO_2 sample. The peak at 400.0 eV demonstrates successful doping of nitrogen.

3 Proposed mechanism that bandgap of the N, Ti^{3+}-TiO_2 are broader than the Ti^{3+}-TiO_2.

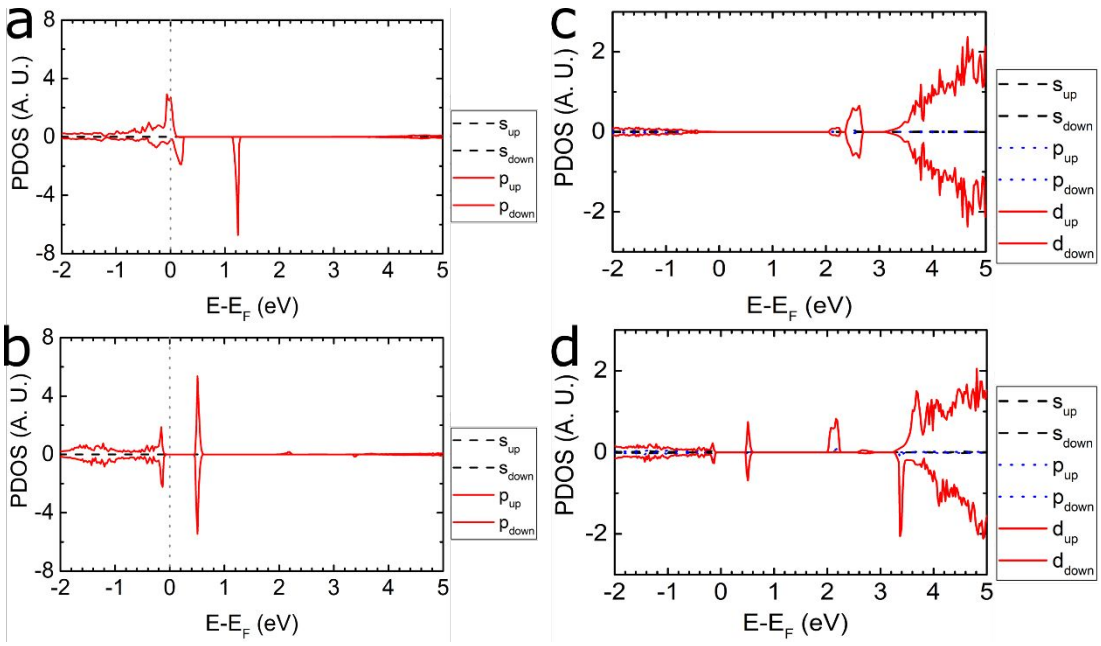

Figure S3. (a, b) Projected density of states (PDOS) of N atom in N-TiO_2 and N, Ti^{3+}-TiO_2, respectively. **(c, d)** PDOS of the nearest Ti atom to N impurities and oxygen vacancy in Ti^{3+}-TiO_2 and N, Ti^{3+}-TiO_2, respectively. Comparing the PDOS of the N impurity in N-TiO_2 (Figure S3a) and N, Ti^{3+}-TiO^2 (Figure S3b), the N 2p orbitals are occupied and shift to lower energy. Meanwhile, the reduction of the features associated Ti^{3+} ions are obvious by comparing the PDOS of the nearest Ti atom to N impurities and oxygen vacancy in Ti^{3+}-TiO_2 (Figure 4c) and N, Ti^{3+}-TiO_2 (Figure 4d). This is because the charge transfers from the high-lying Ti^{3+} 3d orbitals to the low-lying N 2p orbitals, which leads to the shift of the defects states of N defect to lower energy and formation of reoxidized Ti^{4+} ions.

4 Hydrophilic property of Ti^{3+}-TiO_2 sample.

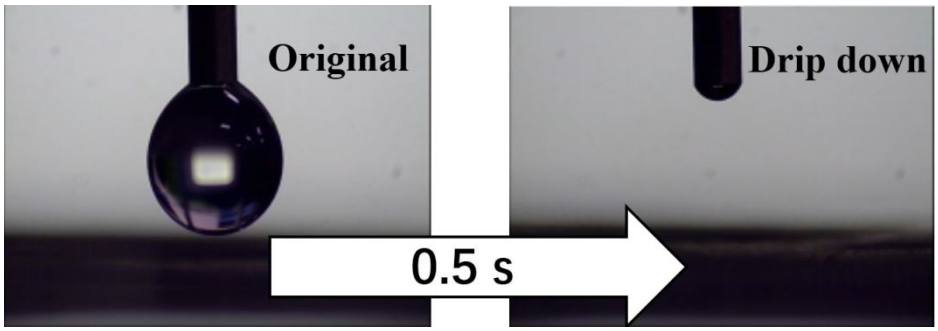

Figure S4. The contact angles of Ti^{3+}-TiO_2 membrane. Shooting interval of camera is set as 0.5 second. The phenomenon that water drop is absorbed by Ti^{3+}-TiO_2 membrane within 0.5 second and contact angle of 0° demonstrate that the Ti^{3+}-TiO_2 membrane is hydrophilic

5 Photo-thermal efficiency calculated in view of energy loss

Table S1. Energy losses.

energy loss	Qoptical	Q1	Q2	Q3	Qtotal
ratio	4.40%	4.30%	2.10%	12.80%	23.60%

$Q_{optical}$

The optical energy losses is represented by 1-α, where α represents the weighted fraction between absorbed radiation energy and incoming solar radiation energy.

$$\alpha = \frac{\int_{200}^{2500} I(\lambda)(1 - R(\lambda))d\lambda}{\int_{200}^{2500} I(\lambda)d\lambda}$$

Where $I(\lambda)$and $R(\lambda)$ are the light intensity function of the solar spectrum and the reflectivity function of the sample at different wavelength. After calculation, α=0.956. The optical energy loss $Q_{optical}$= 1-α= 4.4%.

The heat loss can be divided into three parts named heat conduction loss Q_1, heat convection loss Q_2 and radiation heat transfer loss Q_3.

Q_1

$$Q_1 = \frac{\lambda}{b} A(t_1 - t_0)$$

Where λ is heat conductivity coefficient, b is the thickness of thermal insulator, A is the area of thermal insulator (same as the area of solar absorber), t_1 represents the temperature of solar absorber and t_0 represents the temperature of bulk water. PE foam is utilized as thermal insulator, and the λ is 0.042 W $m^{-1}k^{-1}$, the thickness b is 2 cm, the area A is 28.3 cm^2, the temperature rises from 22 ^oC to 42.7 ^oC, and the calculated Q_1= 0.123 W. And for the absorber with area of 28.3 cm^2 under AM 1.5 sunlight (1000 W m^{-2}), the energy input Q is 2.83 W. The calculated heat conductivity

energy loss Q_1/Q =4.3%.

Q_2

$$Q_2 = -hA(t - t_w)$$

Where h is heat convection coefficient, A is the area of solar absorber, t represents the temperature of airflow and t_w represents the temperature of solar absorber. As for airflow in natural convection condition, the h in air varies from 1-10 W m^{-2} K^{-1}, the surface area A is 28.3 cm^2, the temperature t_w is 42.7 °C and the temperature t is 22 °C. Thus the calculated Q_2 varies from 0.06 W to 0.586 W, the heat convection energy loss Q_2/Q varies from 2.1% to 20.7%

Q_3

$$Q_3 = A\varepsilon\sigma({T_1}^4 - {T_0}^4)$$

Where A is surface area, ε the emissivity of the absorber, σ is the Stefan-Boltzmann constant (5.67×10^{-8} W $m^{-2}K^{-4}$).T_1 represents thermodynamic temperature of solar absorber surface and T_0 represents thermodynamic temperature of room surface. Surface area A is 28.3 cm^2, T_1= 315.85K, T_2=295.15 K. In this work, the Ti^{3+}-TiO_2 shows steadily absorption in solar spectrum in the wavelength from 200 to 2500 nm, and hence it is simplified as gray body with α of 0.956. According to the law of Kirchhoff, the emissivity ε is equal to the absorption rate α when the material is at the condition of thermal equilibrium. The calculated Q_3= 0.362 W, and the radiation heat transfer loss Q_3/Q= 12.8%

Q_{total}

In the view of energy loss, the solar-to-vapor conversion efficiency can be calculated by: $\eta = \frac{Q - (Q_1 + Q_2 + Q_3 + Q_{optical})}{Q}$

The value of η varies from 76.4% to 57.8%. Considering that there is no severe convection in the testing progress, the heat convection coefficient h is set as 1 W m^{-2} K^{-1}, and the result η= 76.4% is similar with the results η= 77.1%.

6 Quality of desalinated water.

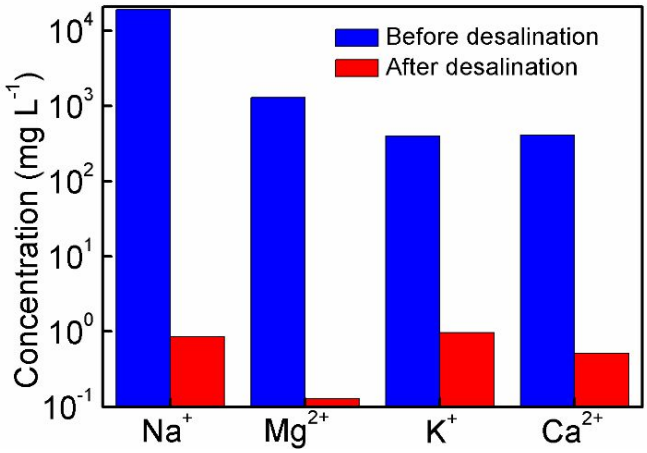

Figure S5. Concentration of main irons (Na+, Mg2+, K+, Ca2+) in the purified water. Concentrations of all ions in desalinated water are far below standard of WHO (170 mg/L) which demonstrates that the purified water meets the requirement of drinking standard.

7 Dispersibility of Ti^{3+}-TiO_2.

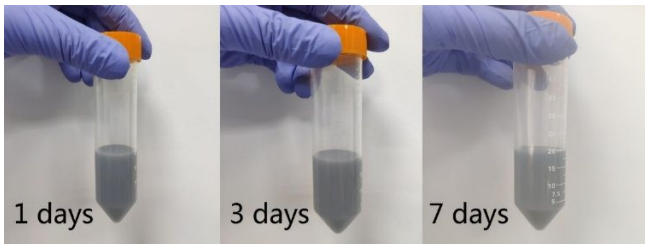

Figure S6. Dispersibility of Ti^{3+}-TiO_2. Concentration of Ti^{3+}-TiO_2 is controlled at 1 mg ml^{-1}. After dispersed in water for 7 days, no obvious sediment can be observed.