Supporting Information

Efficient H2O2 Production from SrTiO3-based Thermoelectrocatalyst for Harvesting Low-Grade Waste Heat

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Sample preparation

All catalyst powders were synthesized by the solid-phase reaction method at 1100 °C for 3 hours. Prior to calcination, stoichiometrically weighed $SrCO_3$, TiO_2 and Nb_2O_3 powders (99.99%, Aladdin Co. Ltd.) were mixed via a wet ball milling process at 300 rpm for 12 hours with ethanol as the medium, followed by drying at 70 °C. To induce oxygen vacancies, the resulting pure $SrTiO_3$ powders were annealed at 800 °C under a flow of mixed H_2/Ar gas (5% H_2 and 95% Ar). The electron doping concentration was adjusted by varying the annealing duration to 9, 12, and 21 hours (hereafter denoted as STO-Ov1, STO-Ov2, and STO-Ov3). In case of Nb substituted $SrTiO_3$ powders, 2 mol%, 5 mol% and 10 mol% of Nb substitution at the Ti site was applied ($SrTi_{1-x}Nb_xO_3$, $x = 0.02, 0.05, 0.1$, hereafter denoted as STNO-0.02, STNO-0.05, and STNO-0.1).
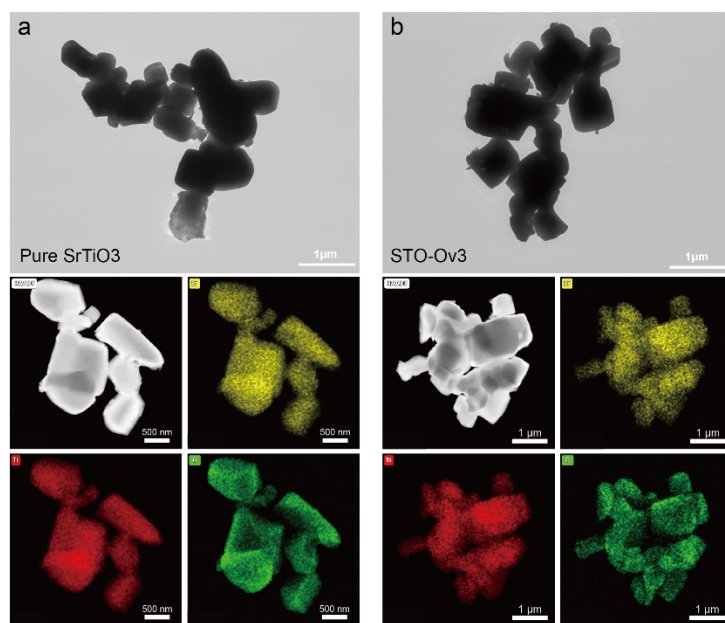

Figure S1. Transmission electron microscopy (TEM) images of $SrTiO_3$ powders before (a) and after (b) post-annealing.

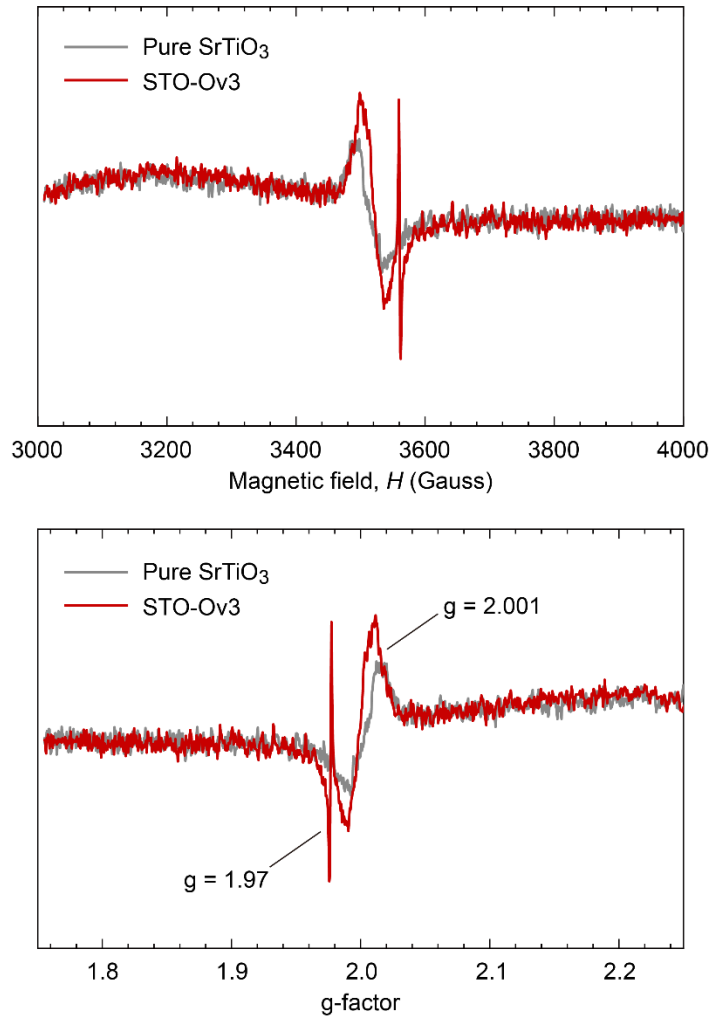**Figure S2. Electron paramagnetic resonance (EPR) spectra of pure SrTiO₃ and STO-Ov3 samples.** EPR signals attributed to oxygen vacancy and Ti^{3+} can be detected at g = 2.001 and 1.97.

Fig. S2 shows the electron paramagnetic resonance (EPR) results of pure $SrTiO_3$ and STO-Ov3 samples. The g factor can be calculated by following relations from magnetic field (*H*),

$$g = hv \, / \, \beta H$$

where *h* is Plank constant (= 6.63×10^{-34} J s), *v* is frequency, *β* is Bohr magneton (9.27×10^{-24} A m²) and H is magnetic field strength.
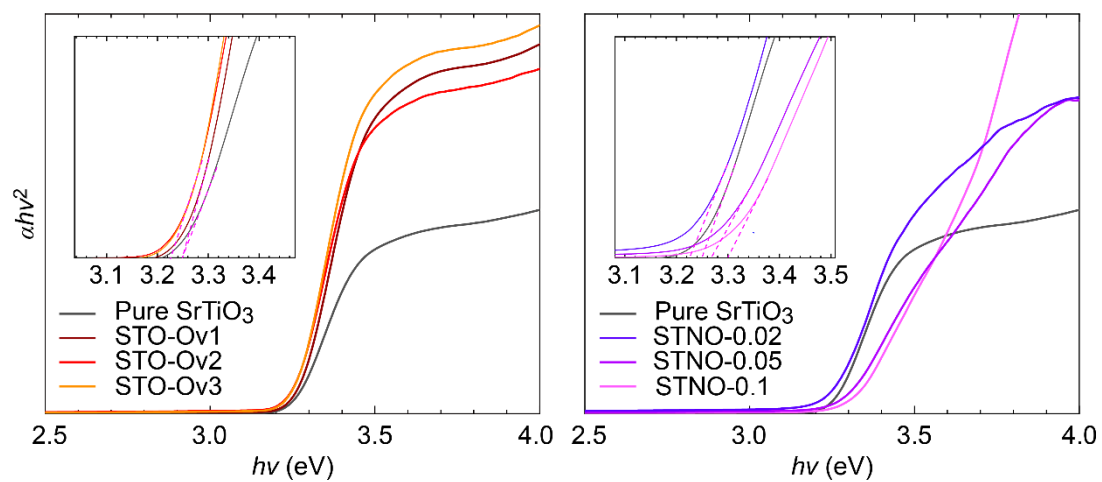
Figure S3. Solid UV characterization of SrTiO$_3$ powders with different oxygen vacancies (Pure-STO, STO-Ov1, STO-Ov2 and STO-Ov3) and Nb substitutions (2 mol%, 5 mol% and 10 mol% substitutions abbreviated as STNO-0.02, STNO-0.05 and STNO-0.1, respectively). All the samples show an almost constant optical band gap of ~3.2 eV, corresponding to the pristine SrTiO$_3$.
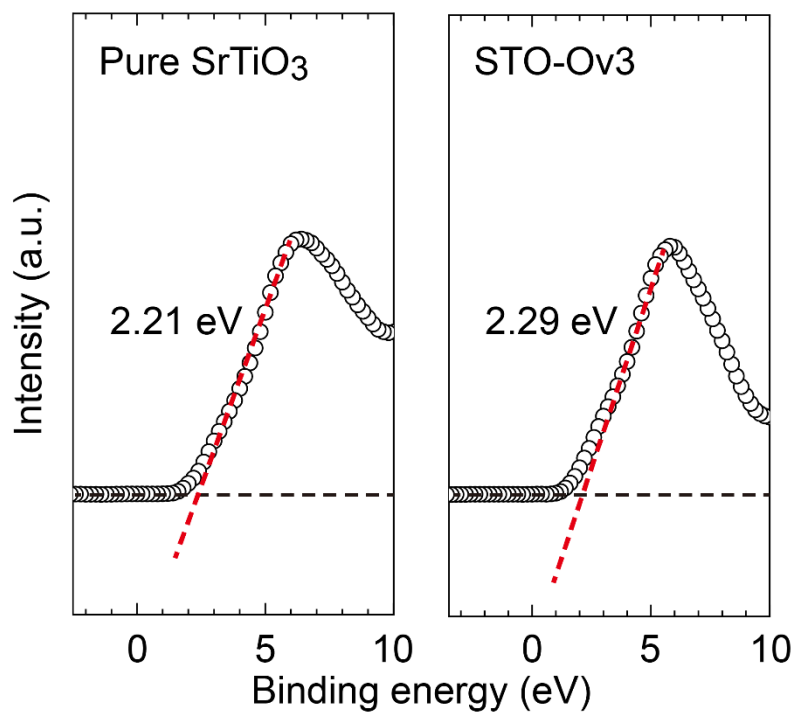
Figure S4. XPS valence band spectra of pure SrTiO₃ and STO-Ov3 powders. The valence band energies are measured to be 2.21 eV for pure $SrTiO_3$ and 2.29 eV for STO-Ov3, showing minimal variation between these two samples.

Table S1. Specific area and porosity of electron doped SrTiO$_3$ powders.

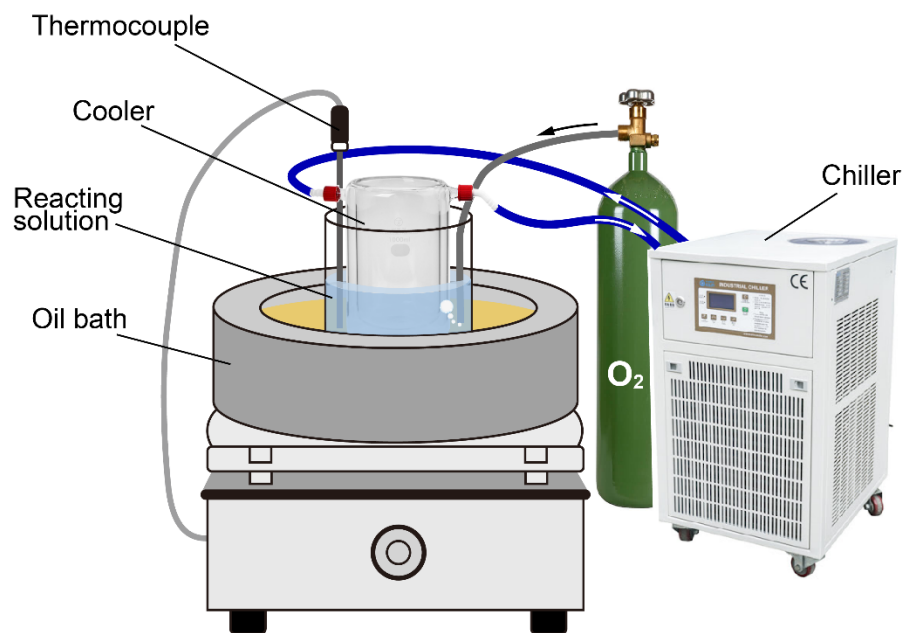| Sample No.	Specific area (m^2 g^{-1})
Pure-SrTiO$_3$	13.57
STO-Ov1	11.93
STO-Ov2	12.08
STO-Ov3	13.63
STNO-0.02	6.87
STNO-0.05	13.99
STNO-0.1	8.11

Figure S5. Schematic illustration of the custom-designed thermoelectrocatalytic (TECatal) reactor.
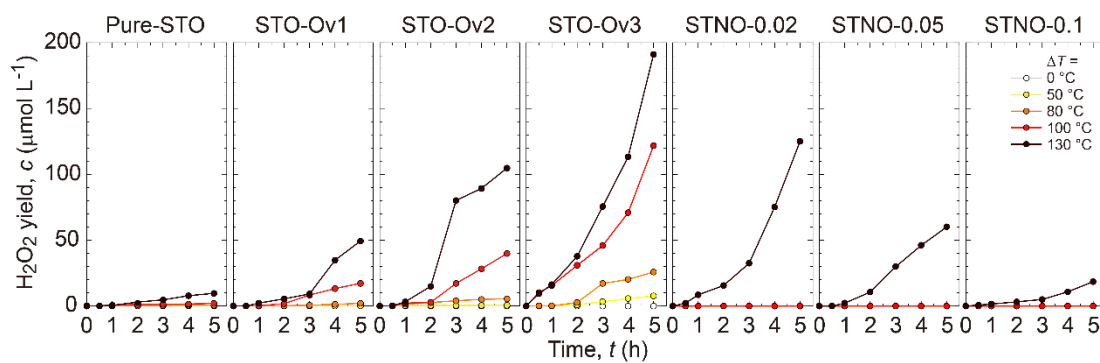
Figure S6. Time-dependent TECatal H_2O_2 production rate of SrTiO$_3$ powders with different oxygen vacancies (Pure-STO, STO-Ov1, STO-Ov2 and STO-Ov3) and Nb substitutions (2 mol%, 5 mol% and 10 mol% substitutions abbreviated as STNO-0.02, STNO-0.05 and STNO-0.1, respectively) at the temperature gradient (ΔT) ranging from 0 to 130 °C.
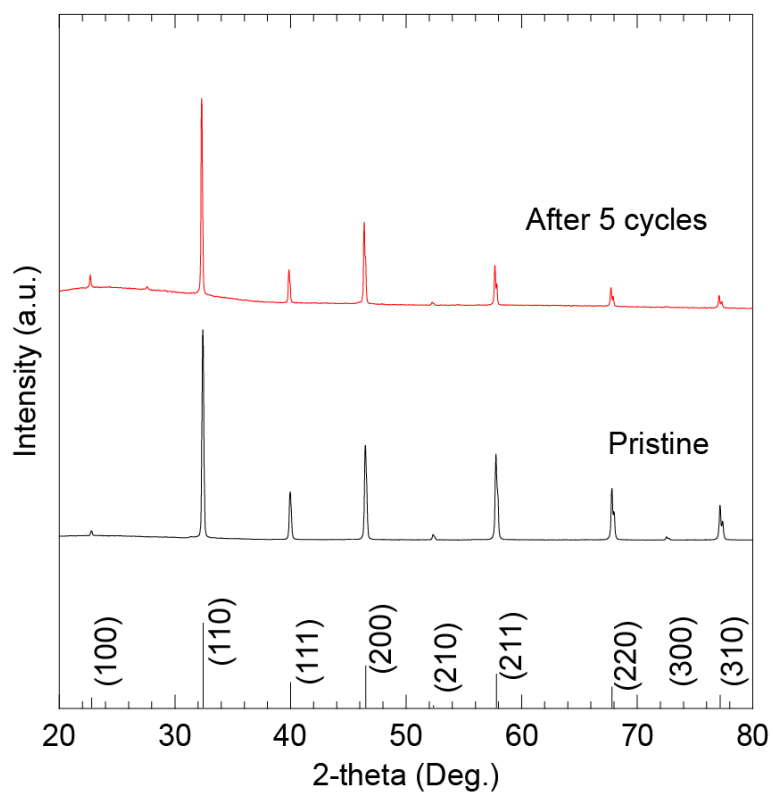
Figure S7. X-ray diffraction (XRD) patterns of oxygen vacancy doped SrTiO₃ powders before and after 5 cycles' thermoelectrocatalysis (TECatal). No obvious phase change can be detected suggesting a good composition stability of $SrTiO_3$ powders.
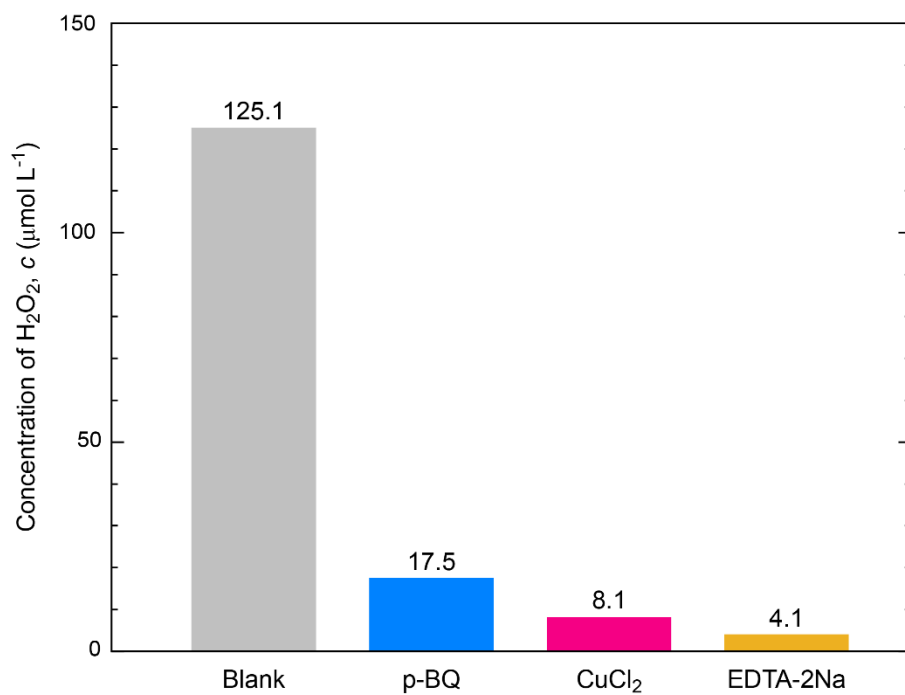
Figure S8. H_2O_2 yield of 2 mol% Nb substituted $SrTiO_3$ powder (STNO-0.02) with EDTA-2Na, $CuCl_2$ and p-benzoquinone (p-BQ) as hole scavenger, electron scavenger and superoxide ($\cdot O_2^-$) scavenger, respectively. Significant suppression of H_2O_2 production can be observed at the presence of scavengers.a