Supporting Information

Exclusive enhancement of catalytic activity in $Bi_{0.5}Na_{0.5}TiO_3$ nanostructures: new insights into the design of efficient piezocatalysts and piezo-photocatalysts

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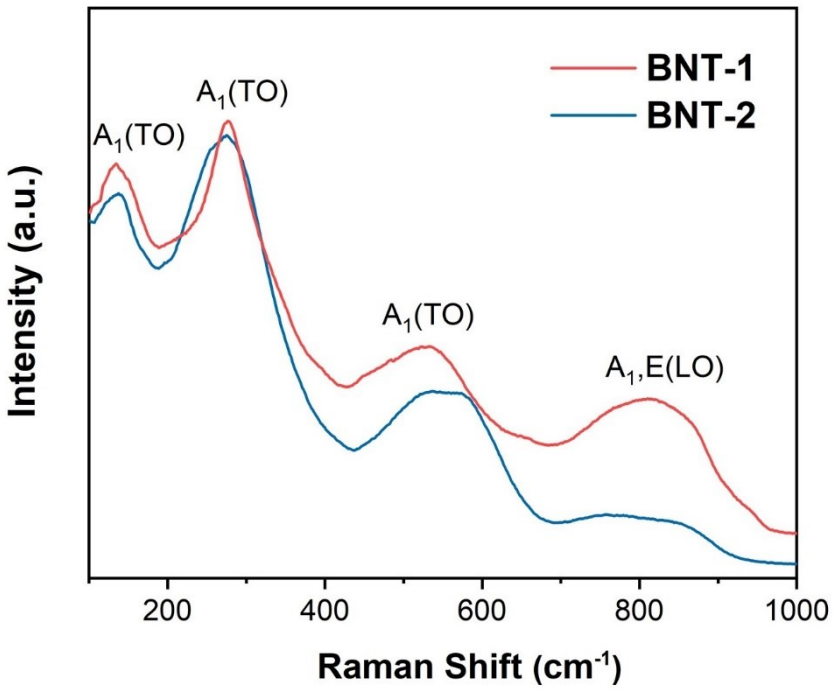

Figure S1. Raman spectra of two different BNT materials.

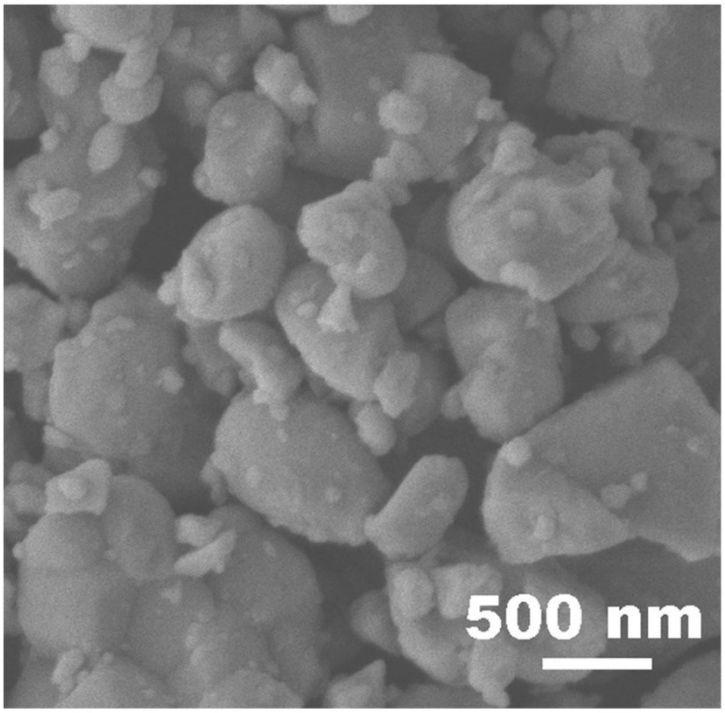

Figure S2. SEM image of BNT-2.

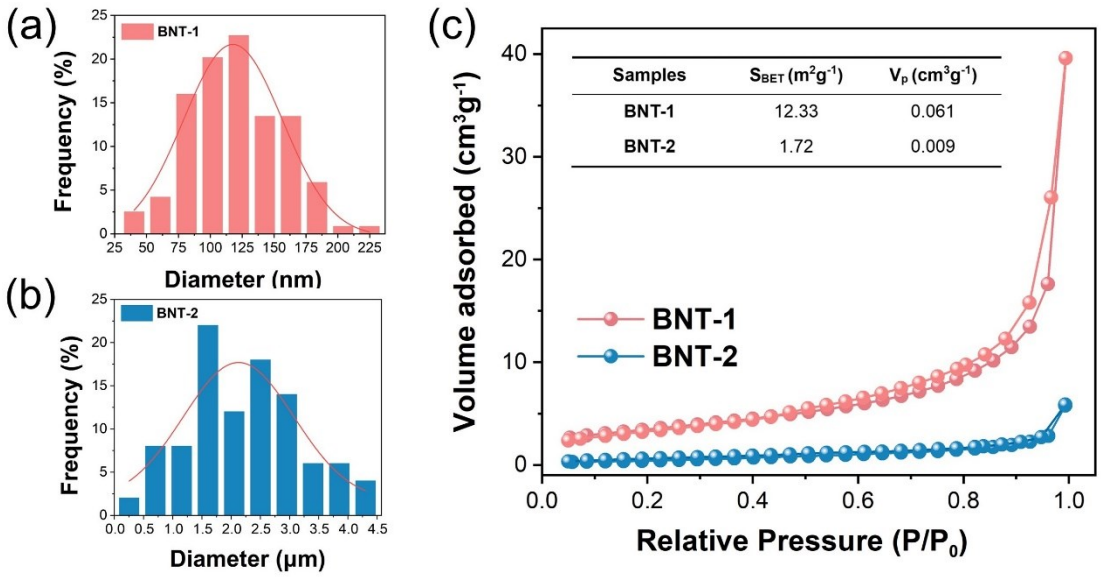

Figure S3. Size distribution histograms of (a) BNT-1 and (b) BNT-2. (c) N_2 adsorption-desorption isotherms of BNT-1 and BNT-2 (inset shows the calculated BET surface area and pore volume).

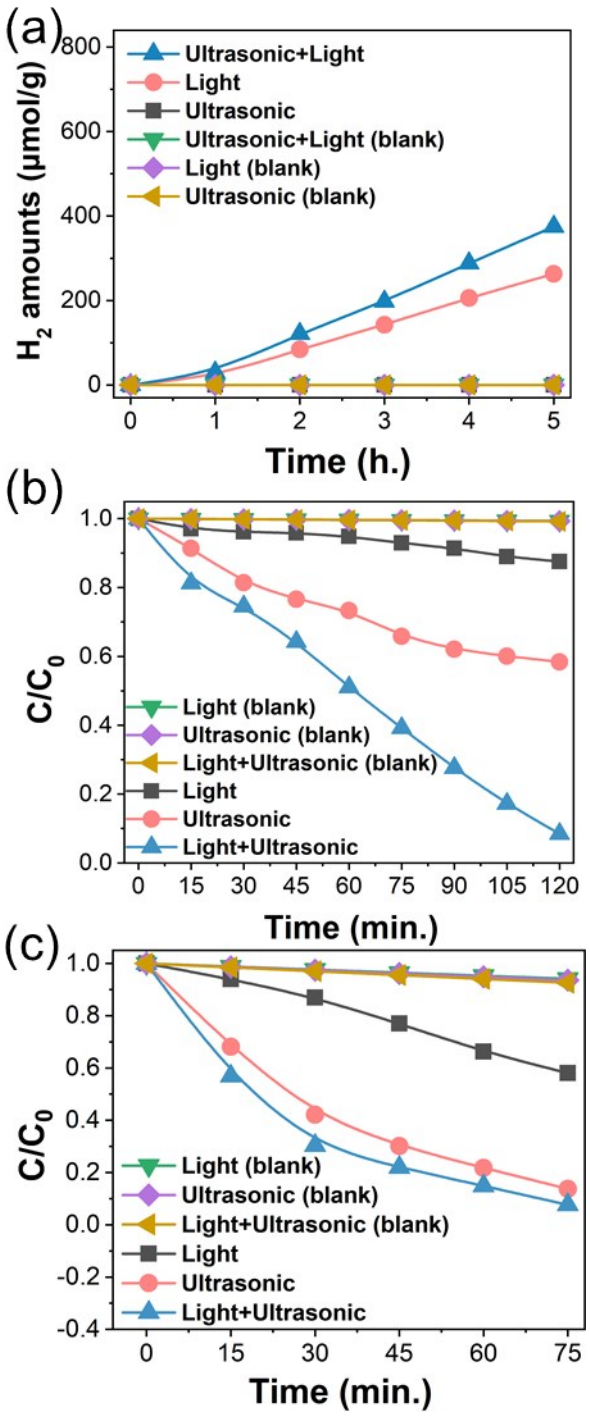

Figure S4. (a) The H_2 production, (b) Cr(VI) reduction and (c) RhB degradation curves with BNT-2 under different conditions.

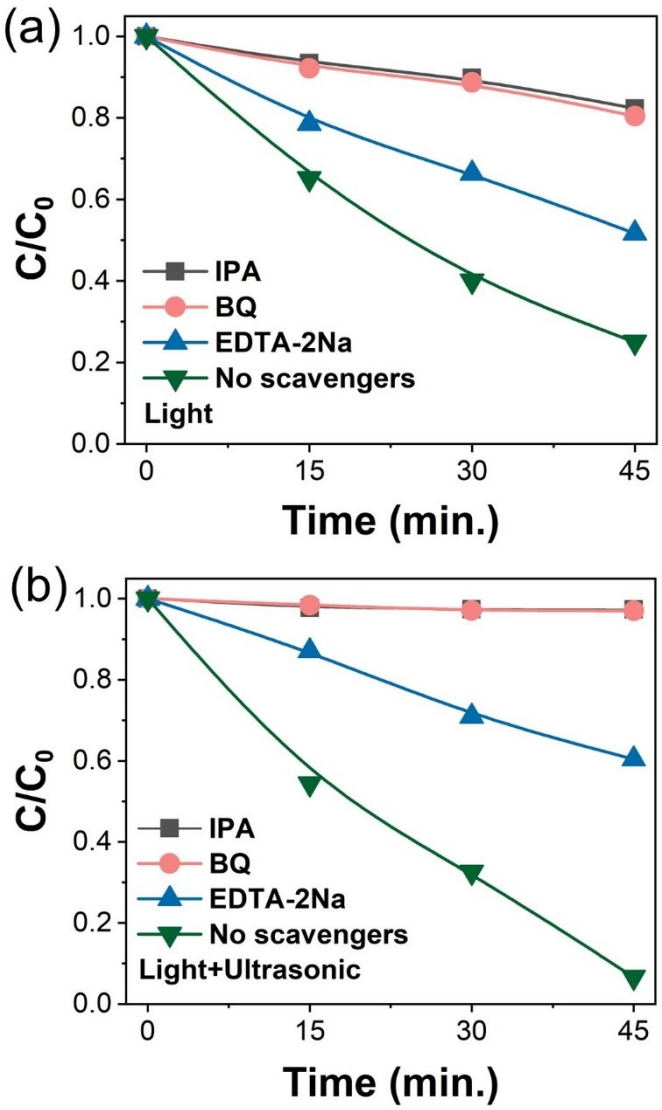

Figure S5. Active-species-trapping experiments for RhB degradation using BNT-1 under (a) light illumination and (b) simultaneous ultrasonic vibration and irradiation by simulated sunlight.

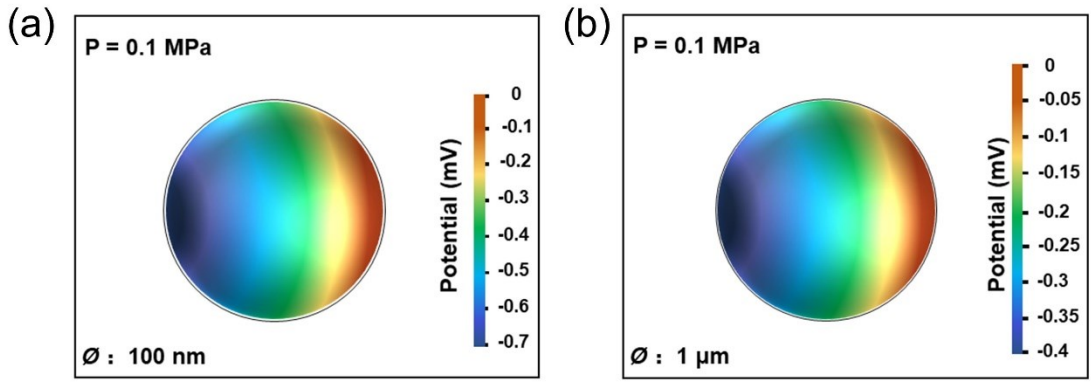

Figure S6. FEM simulation for the piezoelectric potential distribution in (a) BNT-1 and (b) BNT-2 under cavitation pressure of 0.1 MPa, respectively.

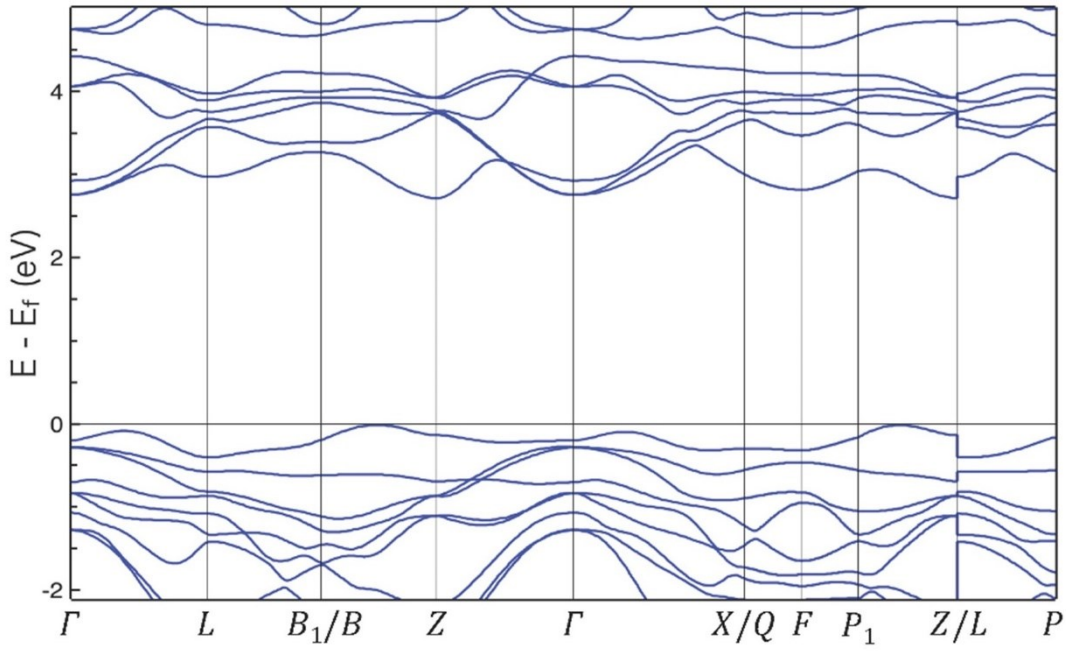

Figure S7. Electronic band structure of bulk BNT at the space group *R*3c. The horizontal solid line indicates the position of the Fermi level.

The first-principles calculations were performed in the framework of density functional theory (DFT). The electronic band gap of the studied materials was obtained via running the Vienna *ab initio* simulation package. The core-valence interactions were treated by the projector augmented wave (PAW) method, where the plane wave expansion was truncated with a cutoff energy of 500 eV. We employed the exchange-correlation functional as the generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) formalism. To better determine the value of band gap, a two dimensional dense k-mesh with a 20 × 20 Monkhorst-Pack grid in momentum space was used in self-consistent calculations.

Table S1. Experimental conditions and first-order rate constants of reported piezoelectric materials.

Catalysts	Catalytic conditions	Catalytic applications	First-order rate constant	Ref.
BNT (nanosphere, ~100 nm)	Ultrasonic (40 kHz, 110 W), room temperature	Degradation of RhB (10 mg L^{-1})	0.0343 min^{-1}	This work
$BaTiO_3$ (nanorod and nanoparticle, ~100-200 nm)	Ultrasonic (40 kHz, 200 W), room temperature	Degradation of RhB (10 mg L^{-1})	0.0044 min^{-1}	[72]
ZnO (nanoparticle, ~20-30 nm)	Ultrasonic (40 kHz, 200 W), room temperature	Degradation of RhB (10 mg L^{-1})	0.0087 min^{-1}	[72]
$NaNbO_3$ (nanowire, ~200 nm in width and ~4 μm in length)	Ultrasonic (40 kHz, 120 W), room temperature	Degradation of RhB (10 mg L^{-1})	0.0161 min^{-1}	[73]

Table S2. The measured electrical conductivity of BNT-1 based bulk sample at room temperature.

Serial number	Resistivity (Ω m)	Conductivity (S/m)
1	72700	1.376E-05
2	72300	1.383E-05
3	72300	1.383E-05
4	72700	1.376E-05
5	72300	1.383E-05

Table S3. Band gap energy variation of BNT under different mechanical force based on DFT calculations.

0 MPa	1 MPa	100 MPa	500 MPa
2.751 eV	2.747 eV	2.745 eV	2.732 eV