Supporting Information

Ultrathin $Ba_{0.75}Sr_{0.25}TiO_3$ nanosheets with highly exposed {001} polar facets for high-performance piezocatalytic application

Kanghui Ke, *Jiang Wu* *, *Zihan Kang*, *Enzhu Lin*, *Ni Qin**, *Dinghua Bao*

State Key Laboratory of Optoelectronic Materials and Technologies, School of Materials Science and Engineering, Sun Yat-Sen University, Guangzhou 510275, China

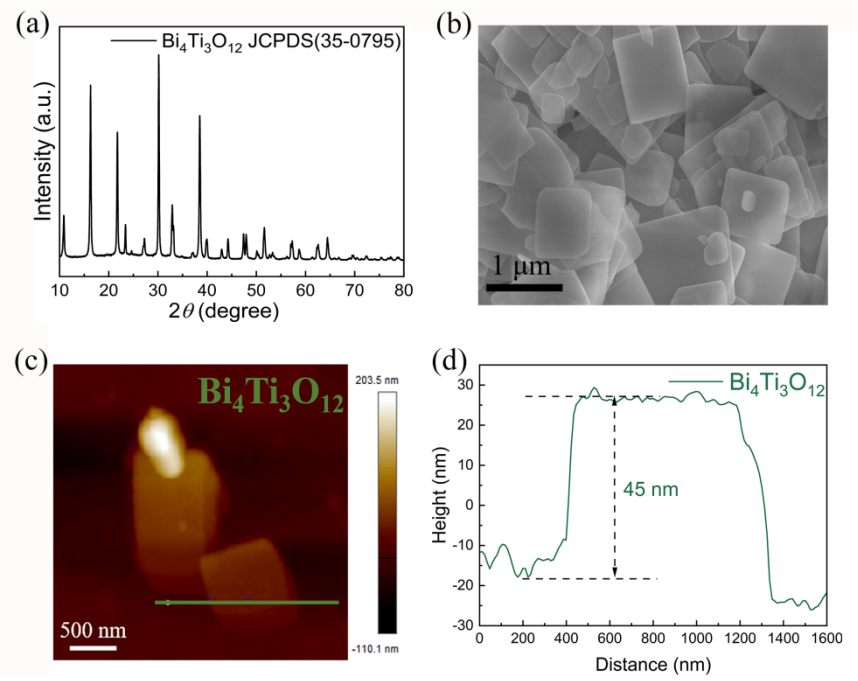

Fig. S1. (a) XRD pattern, (b) SEM image, and (c) AFM image of the $Bi_4Ti_3O_{12}$ nanoplates as synthesized by molten salt method. (d) Height profile of a single $Bi_4Ti_3O_{12}$ nanoplate along the green line in the AFM image.

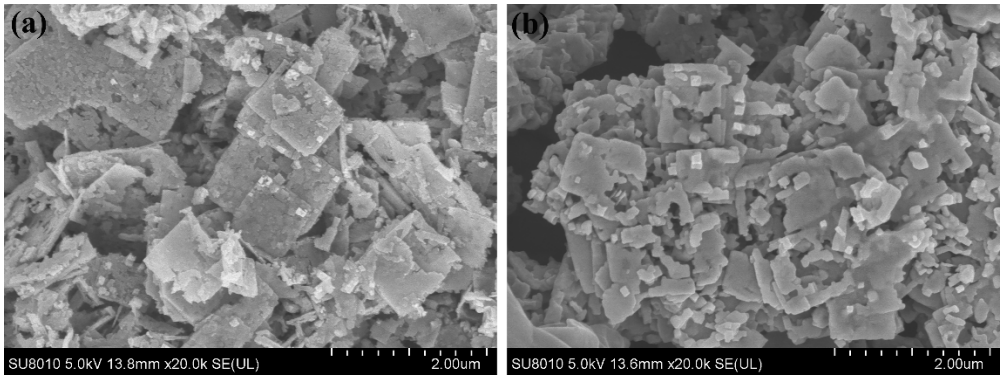

Fig. S2. SEM images of the synthesized (a) $Ba_{0.85}Sr_{0.15}TiO_3$ and (b) $Ba_{0.7}Sr_{0.3}TiO_3$.

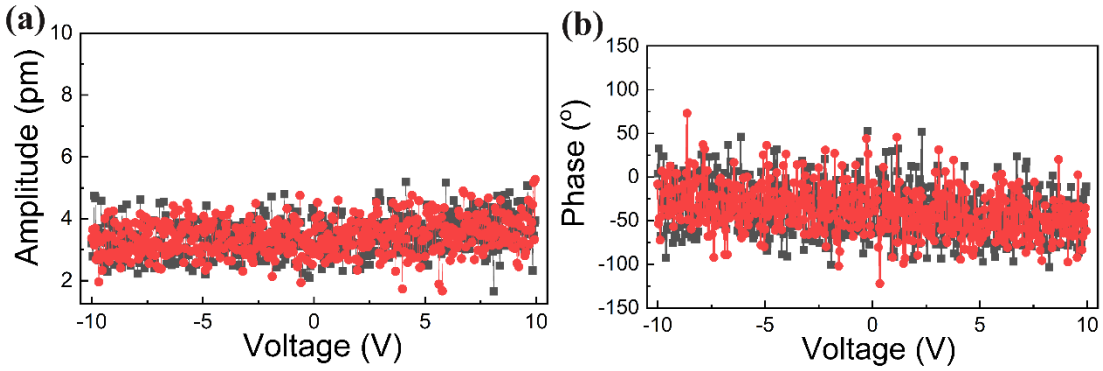

Fig. S3. In-plane (a) amplitude butterfly loop and (b) phase hysteresis loop of the prepared $Ba_{0.75}Sr_{0.25}TiO_3$.

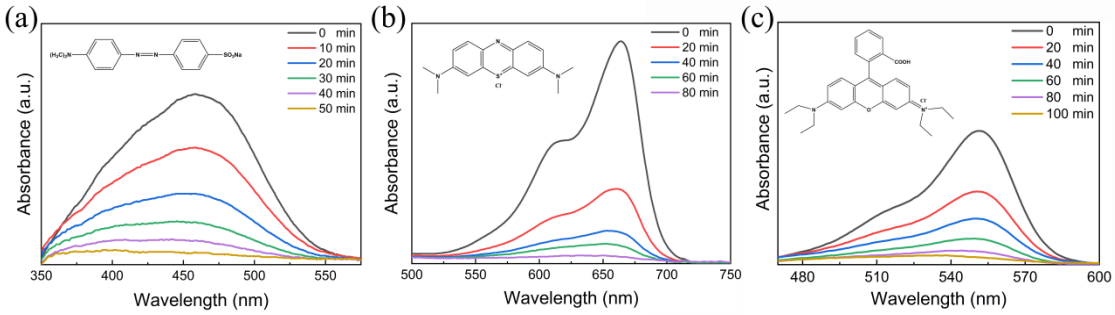

Fig. S4. Evolution of UV-vis absorption spectra of (a) MO, (b) MB and (c) RhB solutions during the piezocatalytic degradation using $Ba_{0.75}Sr_{0.25}TiO_3$ nanosheets as piezocatalyst.

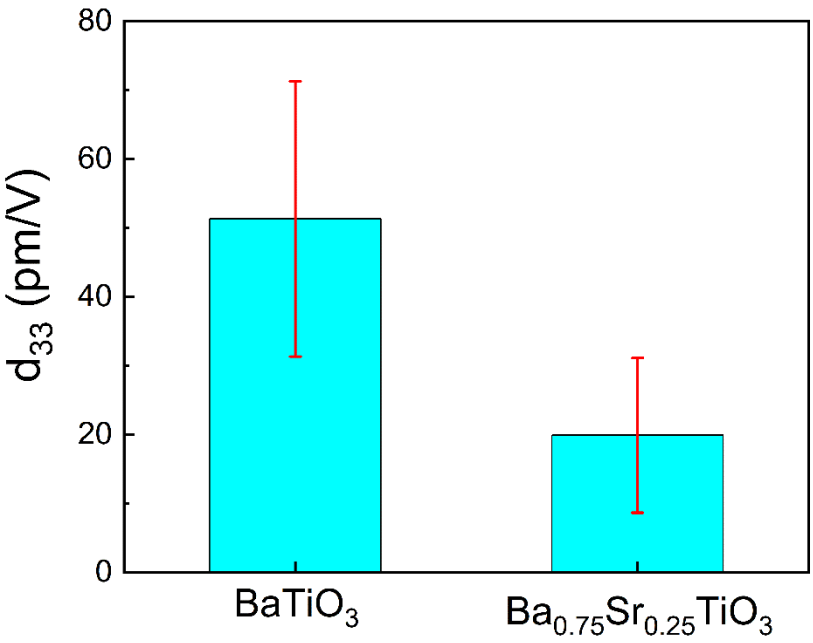

Fig. S5. d_{33} of the synthesized $BaTiO_3$ and $Ba_{0.75}Sr_{0.25}TiO_3$.

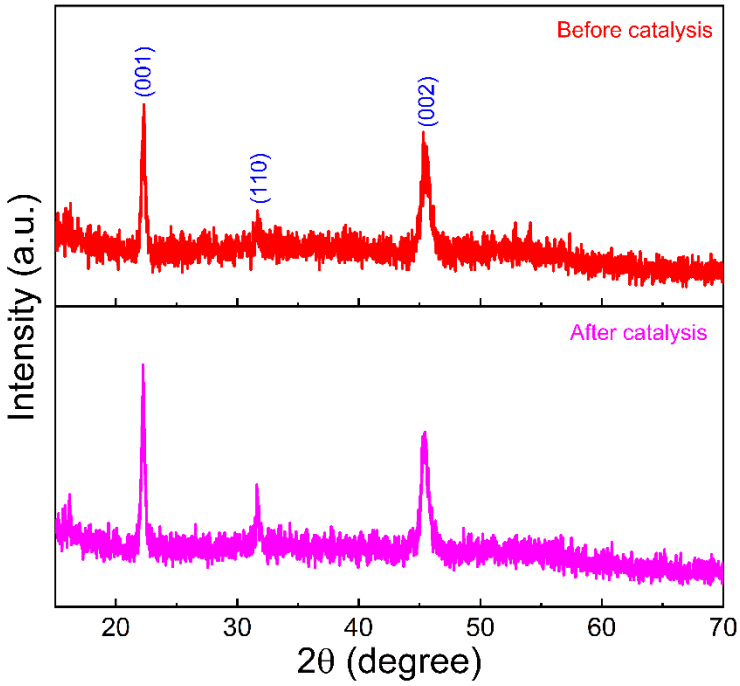

Fig. S6. XRD patterns of the $Ba_{0.75}Sr_{0.25}TiO_3$ before and after cyclic test.

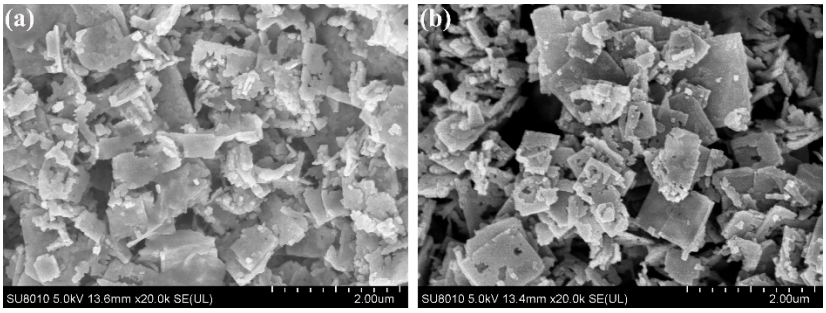

Fig. S7. SEM images of the (a) pristine and (b) recycled $Ba_{0.75}Sr_{0.25}TiO_3$.

DFT Calculation

The spin-polarized density functional theory (DFT) calculations were conducted by using the projected augmented wave (PAW) pseudopotentials [1], as implemented in the Vienna ab-initio Simulation Package (VASP) [2,3]. The exchange correlation function of Perdew-Burke-Ernzerhof (PBE) form was employed [4], with a plane wave basis cut-off energy set to 450 eV. The convergence criteria were set to be 10^{-4} in energy and 0.02 eV/Å in force. The $BaTiO_3$ and $Ba_{0.75}Sr_{0.25}TiO_3$ with the BaO-terminated (001) surface was modelled by a seven-layer slab, where the atoms in the bottom three layers were fixed at the theoretical bulk lattice positions. The Brillouin zone was sampled by a Monkhorst–Pack k-point mesh of 4×4×1 grid and a vacuum layer of 15 Å was employed to avoid interactions of neighboring images. The van der Waals (vdW) interactions between $BaTiO_3$ and reactants were treated using the Grimme's D3-type of the semiempirical method [5].

Adsorption energies (E_{ads}) were calculated by using the following equation.

$$E_{ads} = E_{total} - E_{substrate} - E_{reactant}$$

where E_{total} is the total energy of adsorbed systems, $E_{substrate}$ and $E_{reactant}$ are the energies of the substrate $BaTiO_3$/$Ba_{0.75}Sr_{0.25}TiO_3$ and reactants, respectively. According to the definition, a negative E_{ads} indicates an energetically stable configuration.

References

1. P. E. Blöchl, Phys. Rev. B 50, (1994) 17953-17979.
2. G. Kresse, J. Furthmüller, Phys. Rev. B 54 (1996) 11169-11186.
3. G. Kresse, J. Hafner, Phys. Rev. B 49 (1994) 14251-14269.
4. J. P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 77 (1996) 3865-3868.
5. S. Grimme, J. Antony, S. Ehrlich, H. Krieg, J. Chem. Phys. 132 (2010) 154104.