Supplementary information

Hydrogen production by photocatalytic water splitting of aqueous hydrogen iodide over Pt/alkali metal tantalates

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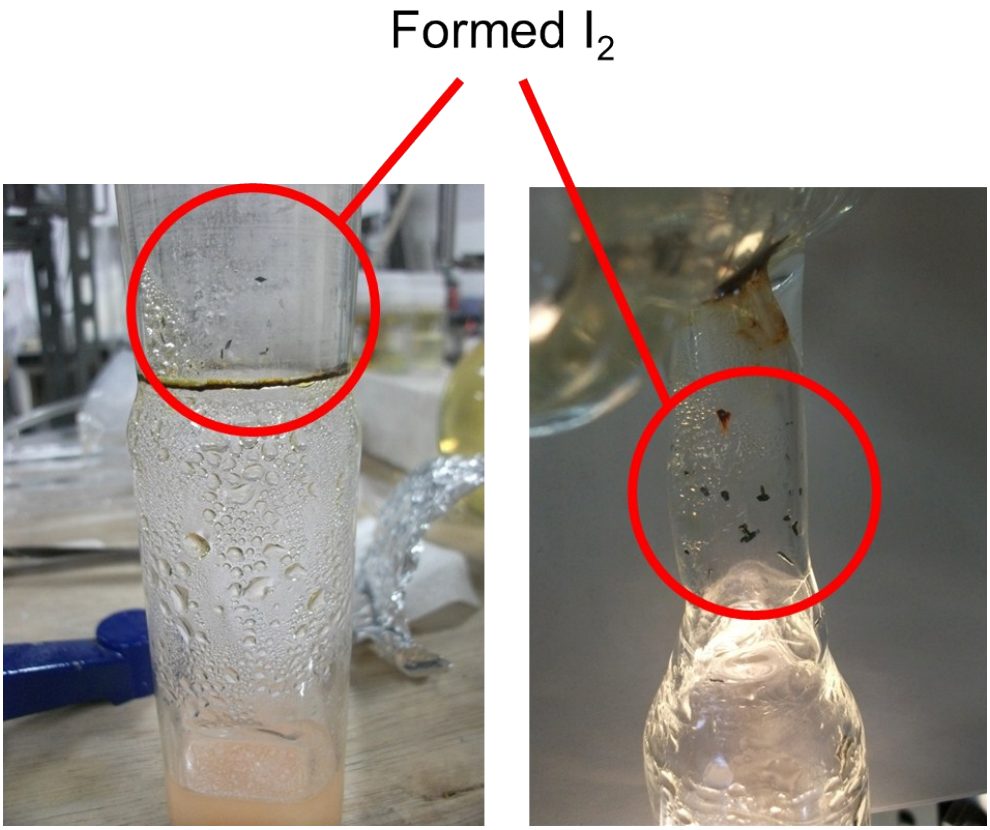

Fig. S1 Photographs of quartz cell after photocatalytic hydrogen iodide decomposition reaction. Light source: 500 W Xe lamp (full arc, 2.0 W cm^{-2}); reaction time: 12 h; photocatalyst: Pt (0.2 wt%)/$KTaO_3$; reactor type: bacth type reactor.

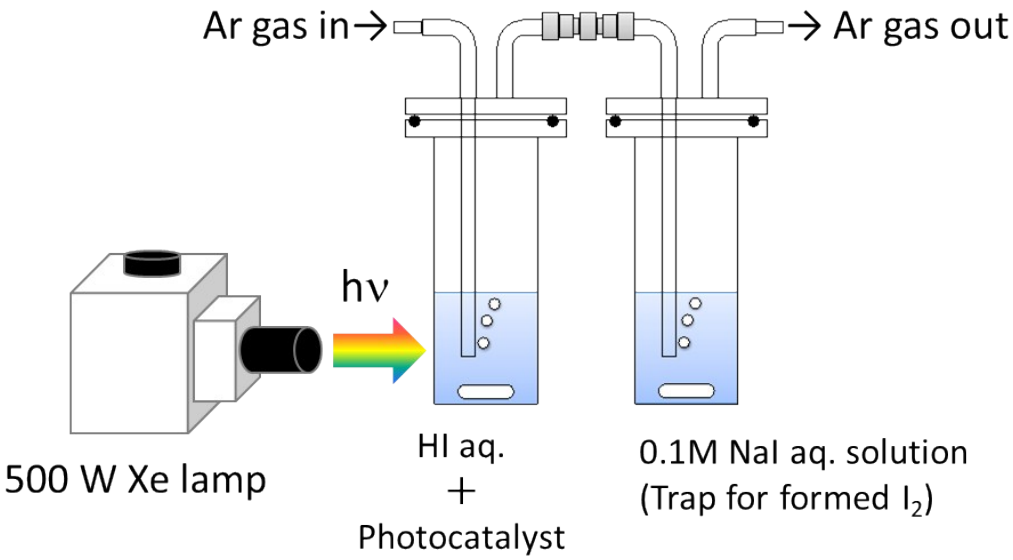

Fig. S2 Schematic image of flow type reactor for photocatalytic HI decomposition in this study. Light source: 500 W Xe lamp (full arc, 2.0 W cm^{-2}); reaction time: 6 h; reaction solution: 0.1 M HI aqueous solution (30 ml); Amount of photocatalyst: 50 mg; Ar flow rate: 50 ml/min.

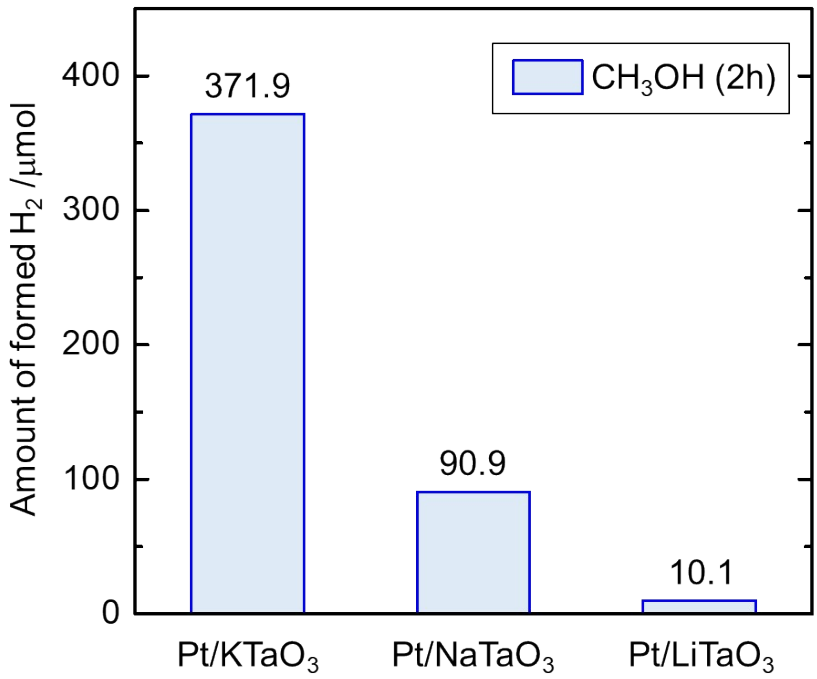

Fig. S3 Amounts of H_2 formed from aqueous methanol solution over Pt/$ATaO_3$ photocatalysts. Light source: 500 W Xe lamp (full arc, 2.0 W cm^{-2}); reaction time: 2 h; reaction solution: 50 vol.% aqueous methanol solution (30 ml); Amount of photocatalyst: 50 mg.

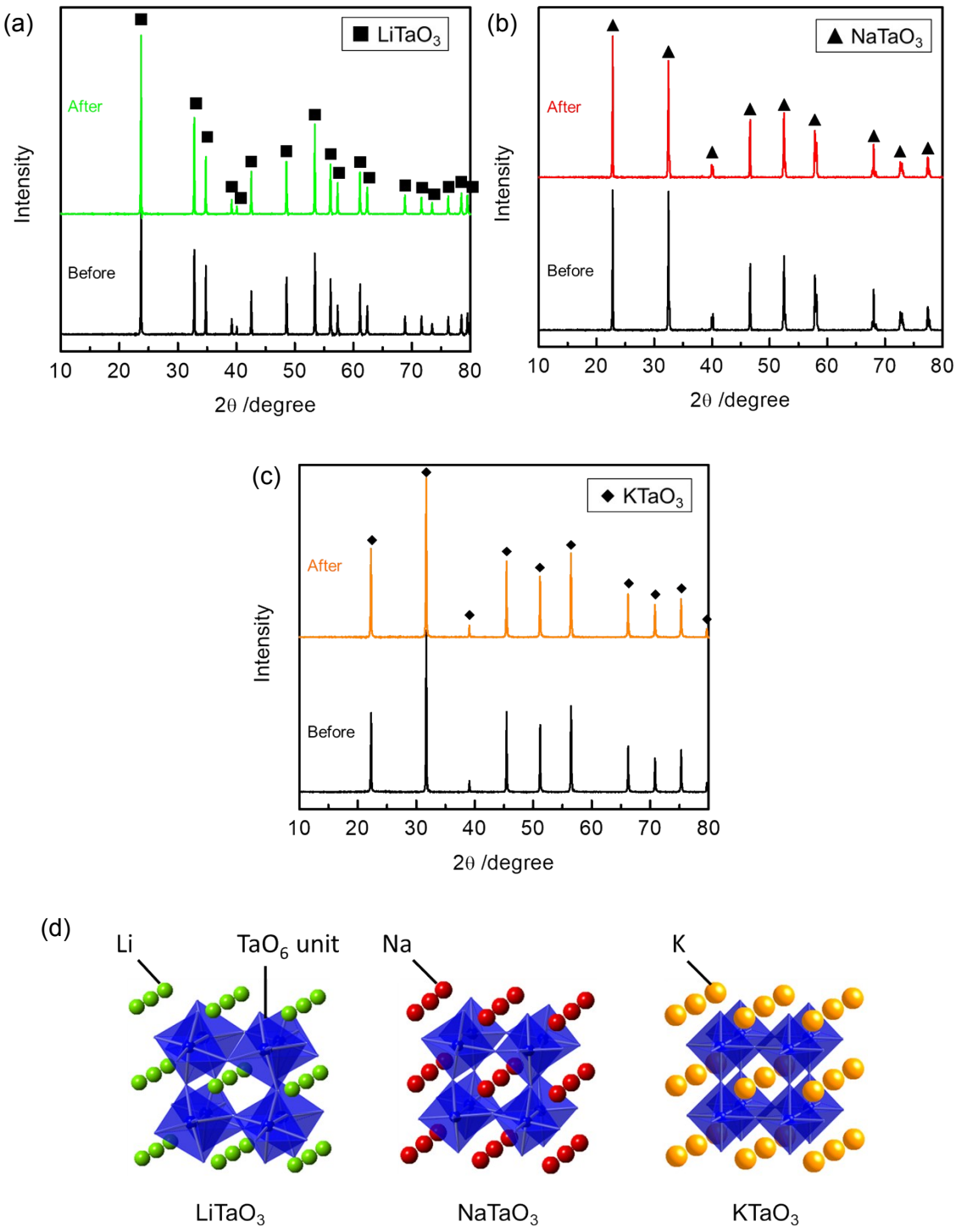

Fig. S4 XRD patterns of (a) $LiTaO_3$, (b) $NaTaO_3$, and (c) $KTaO_3$ before and after HI photodecomposition reaction. (d) Crystal structures of $ATaO_3$ (A: Li, Na, K).

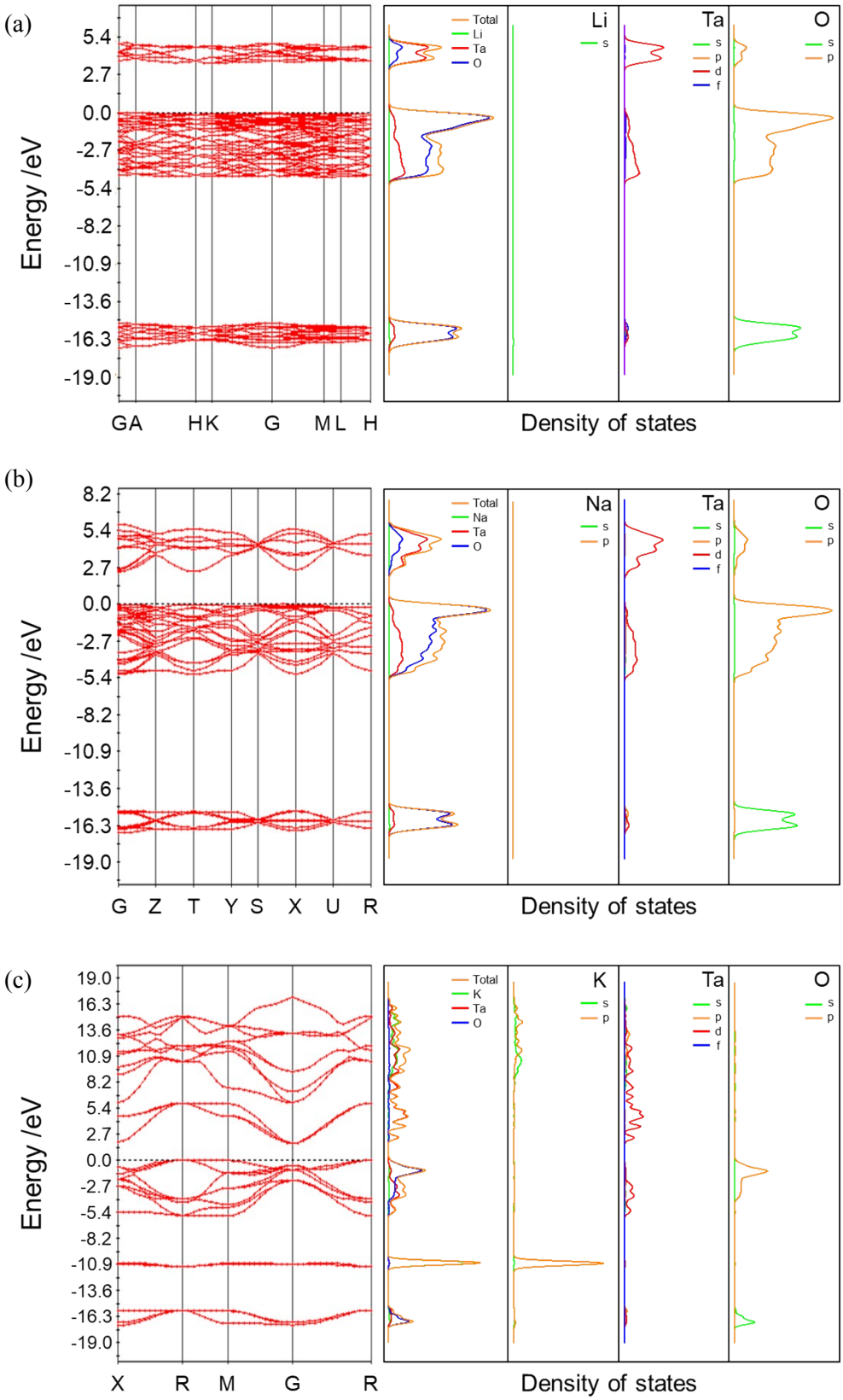

Fig. S5 Calculated band structures, total density of states, partial density of states of constituent elements of (a) $LiTaO_3$, (b) $NaTaO_3$ and (c) $KTaO_3$.

Theoretical calculations

The electronic structures of $ATaO_3$ (A: Li, Na, K) was studied by theoretical calculation using DFT implemented in the DMol^3 software package. The generalized gradient approximation with Perdew-Burke-Ernzerhof functional was used to describe the exchange-correlation interaction. All electrons were treated in this caluculation. The convergence criteria for energy, maximum force, and displacement were set as 1×10^{-5} Ha, 0.002 Ha/Å, and 0.005 Å, respectively. Static calculations were carried out using a Monkhorst-Pack k-point grid, $3 \times 3 \times 2$ for $LiTaO_3$, $3 \times 2 \times 3$ for $NaTaO_3$ and $4 \times 4 \times 4$ for $KTaO_3$.

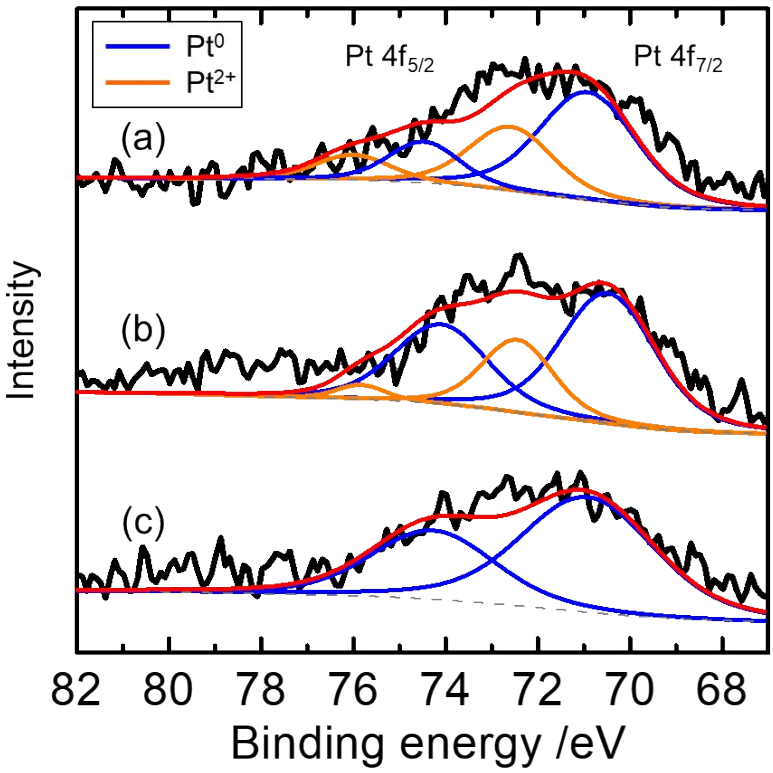

Fig. S6 XPS spectra of Pt cocatalysts on (a) $KTaO_3$, (b) $NaTaO_3$, and (c) $LiTaO_3$ after photocatalytic HI decomposition

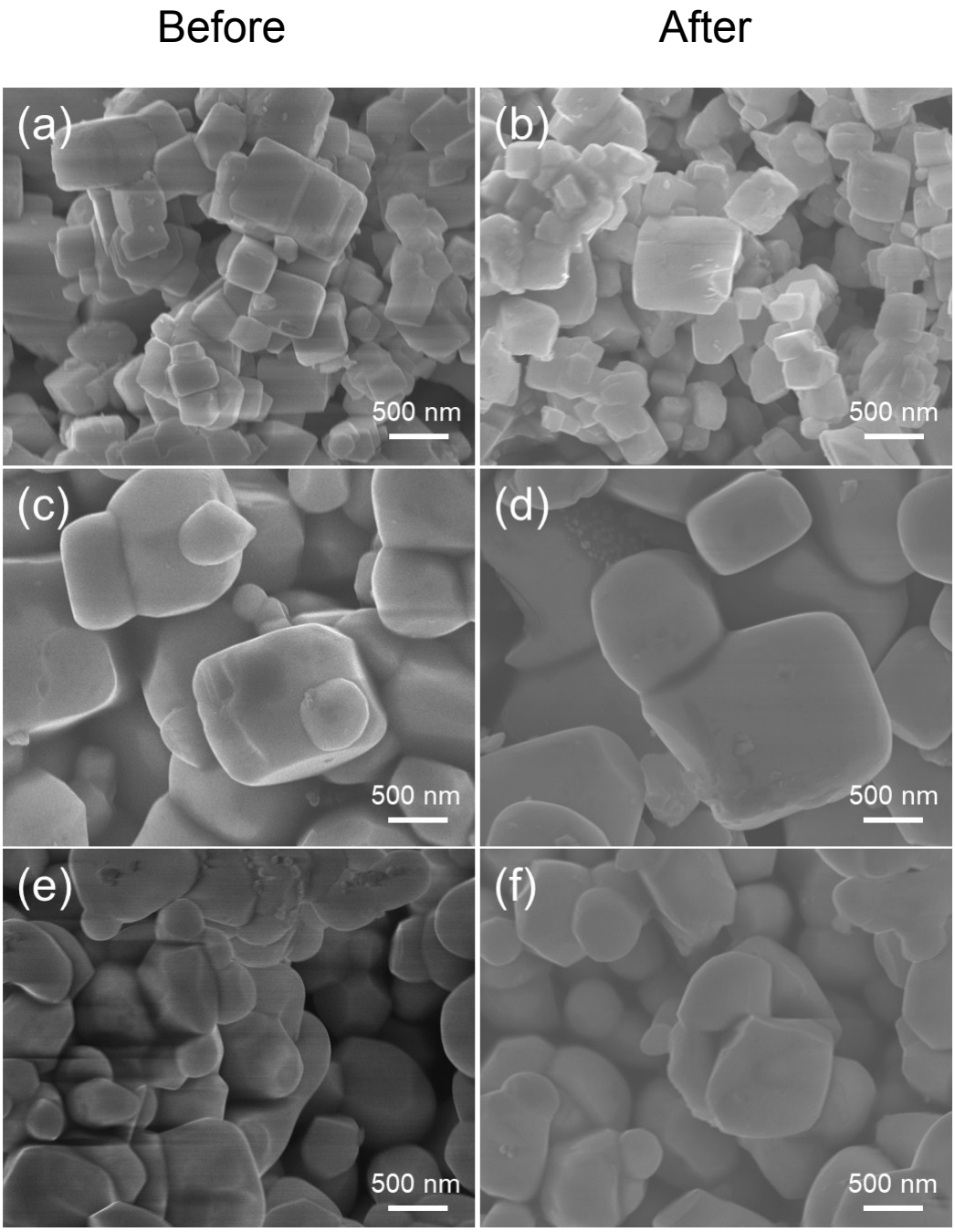

Fig. S7 SEM images of (a)(b) Pt/$KTaO_3$, (c)(d) Pt/$NaTaO_3$, (e)(f) Pt/$LiTaO_3$ before and after photocatalytic reaction.