

Supporting Information

Nature of Catalytic Active Sites Present on the Surface of Advanced Bulk Tantalum Mixed Oxide Photocatalysts

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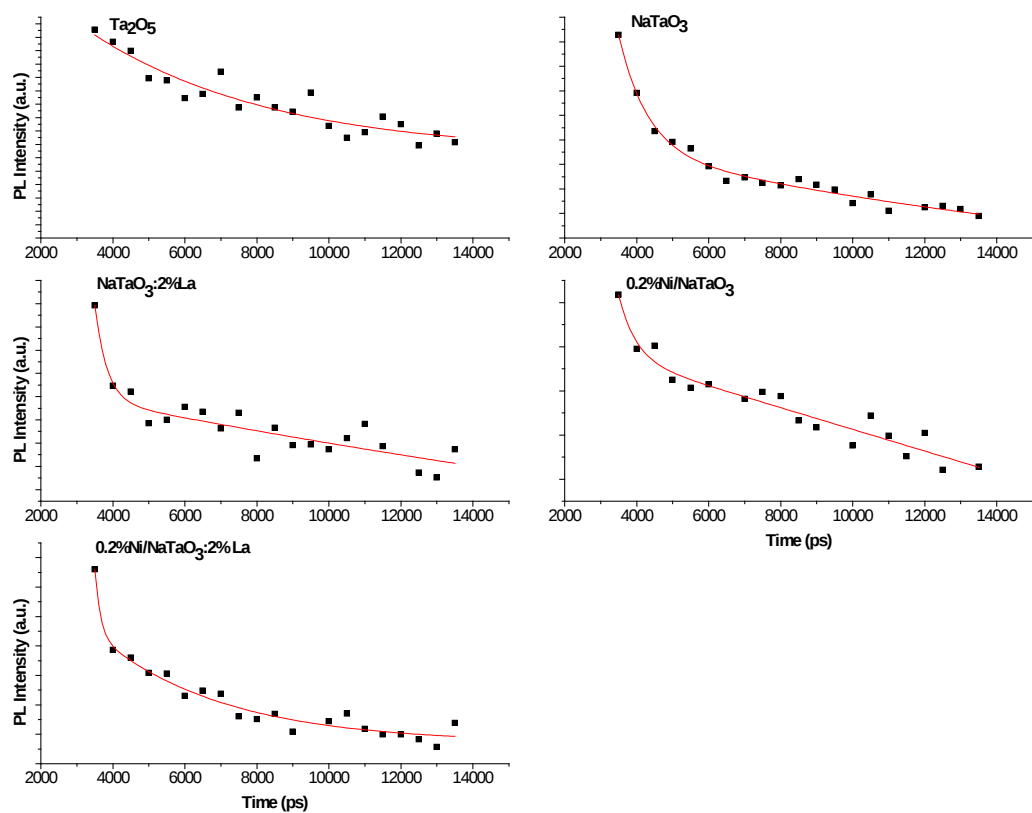


Figure S1. PL emission decay curves for tantalum-based photocatalysts.

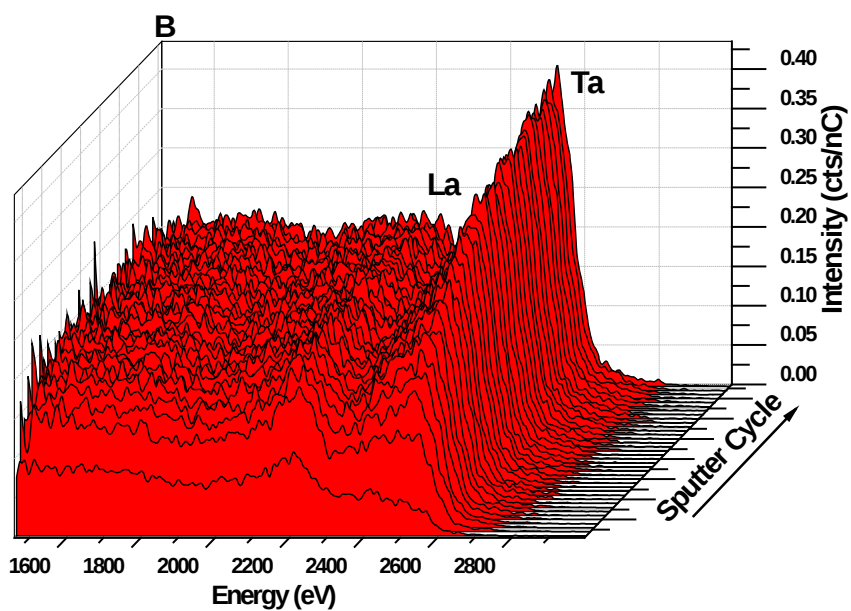
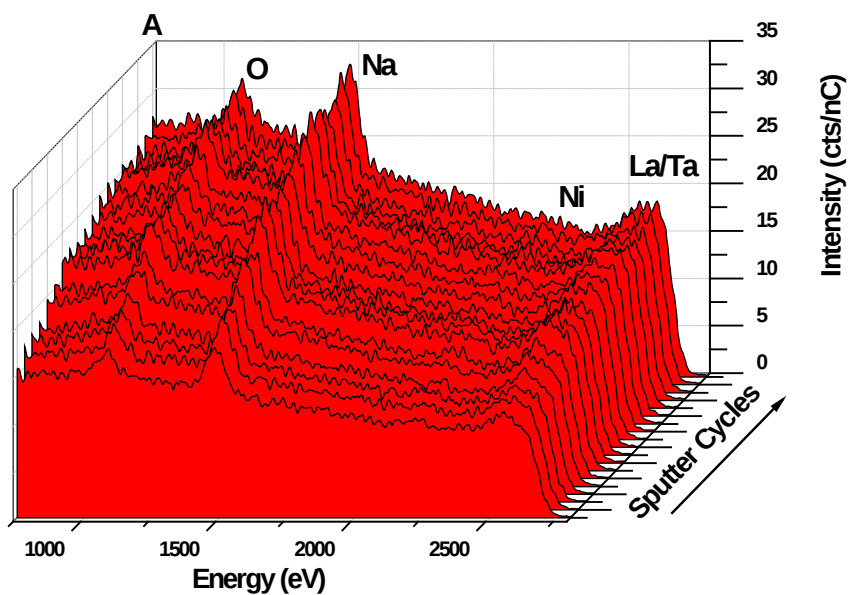


Figure S2. HS-LEIS depth profile for the promoted 0.2%NiO/NaTaO₃:2%La photocatalyst using (A) He⁺ ion gas and (B) Ne⁺ ion gas.

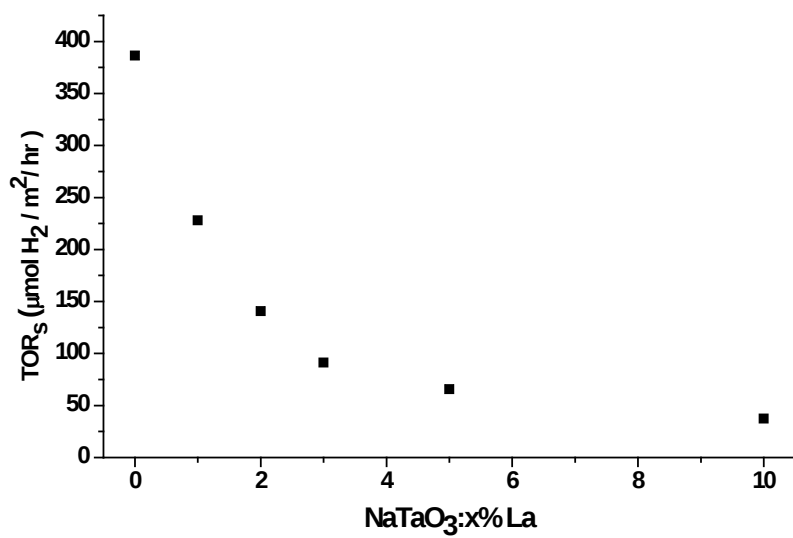


Figure S3. TOR_s (micromoles of H₂ per square meter per hour) as a function of La loading for NaTaO₃:La.

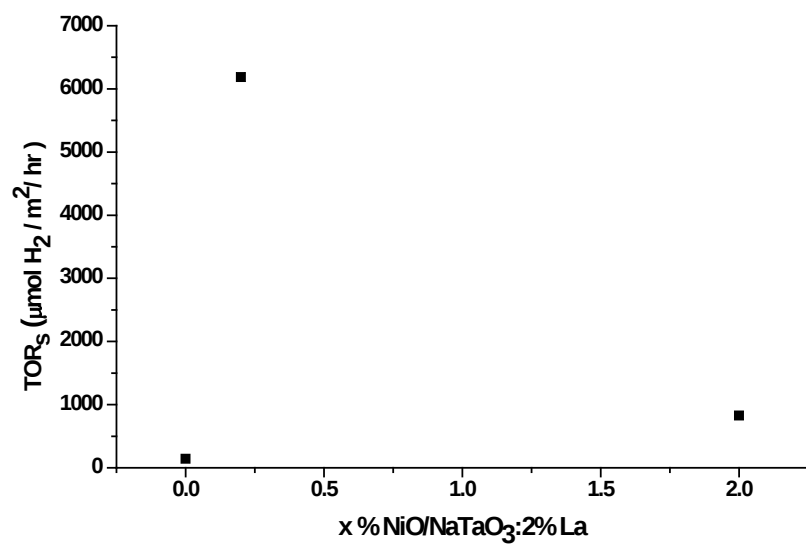


Figure S4. TOR_s (micromoles of H₂ per square meter per hour) as a function of Ni loading for NaTaO₃:2%La.

Calculation of N_s for $\text{NaTaO}_3:2\%\text{La}$:

XPS atomic concentration Ta = 13.4 % (1-3 nm)

30% XPS signal from outermost surface layer (Scienta ESCA-300 instrument surface sensitivity)

Ta Outermost surface concentration $\approx 0.3 * 13.4\% \approx 4.02\%$

$$\text{NaTaO}_3:2\%\text{La} \approx 1 \times 10^{15} \frac{\text{atoms}}{\text{cm}^2}$$

$$N_s = .0402 * 1 \times 10^{15} \frac{\text{Ta atoms}}{\text{cm}^2} * \frac{(100\text{cm})^2}{\text{m}^2} * 3.2 \frac{\text{m}^2}{\text{g}} = \frac{1.3 \times 10^{18} \text{ Ta sites}}{\text{g NaTaO}_3:2\%\text{La}}$$

Calculation of N_s for $0.2\%\text{NiO}/\text{NaTaO}_3:2\%\text{La}$ (similar procedure for $0.05\%\text{NiO}/\text{NaTaO}_3$)

Ni signal (HS-LEIS) of outermost surface layer estimated at $\approx 25\%$ of total Ni since Ni dispersed both on outermost surface and ~ 8 layers below the surface.

Mass NiO = 0.002 g

$$\begin{aligned} N_s &= 0.002 \text{ g} \frac{1}{74.69 \frac{\text{g NiO}}{\text{mol NiO}}} * \frac{6.02 \times 10^{23} \text{ molecules NiO}}{\text{mol NiO}} * 0.25 \\ &= \frac{4.0 \times 10^{18} \text{ NiO sites}}{\text{g } 0.2\%\text{NiO}/\text{NaTaO}_3:2\%\text{La}} \end{aligned}$$