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## Supporting information

Table 1. BVS results of the independent Nb and V atoms in compounds $\mathbf{1}$ and $\mathbf{2}$.

| $\mathrm{Compound} \mathbf{1}$ |  |
| :--- | :--- |
| $\mathrm{Nb}(1)$ | 5.05 |
| $\mathrm{Nb}(2)$ | 5.19 |
| $\mathrm{Nb}(3)$ | 4.92 |
| $\mathrm{Nb}(4)$ | 4.25 |
| $\mathrm{Compound} \mathbf{2}$ | 5.00 |
| $\mathrm{Nb}(1)$ | 4.93 |
| $\mathrm{Nb}(2)$ | 4.94 |
| $\mathrm{Nb}(3)$ | 4.99 |
| $\mathrm{Nb}(4)$ | 4.89 |
| $\mathrm{Nb}(5)$ | 4.98 |
| $\mathrm{Nb}(6)$ | 4.96 |
| $\mathrm{Nb}(7)$ | 4.97 |
| $\mathrm{Nb}(8)$ | 4.93 |
| $\mathrm{Nb}(9)$ | 4.92 |
| $\mathrm{Nb}(10)$ | 4.91 |
| $\mathrm{Nb}(11)$ | 4.93 |
| $\mathrm{Nb}(12)$ | 5.24 |
| $\mathrm{~V}(1)$ | 5.12 |
| $\mathrm{~V}(2)$ | 4.54 |
| $\mathrm{~V}(3)$ | T |
| T |  |

The equations used for the BVS of Nb are $\mathrm{s}=\exp [(1.911-\mathrm{r}) / 0.37]$, while the equations used for the BVS of V are $\mathrm{s}=\exp [(1.803-\mathrm{r}) / 0.37] .{ }^{1}$ The BVS of $V(3)$ is relatively lower than those of $V(1)$ and $V(2)$, which is caused by the disorder of $\mathrm{V}(3)$.


Fig. s1. IR spectra of compounds $\mathbf{1}$ and $\mathbf{2}$.


Fig. s2. Experimental and simulated XRD patterns of compounds $\mathbf{1}$ and $\mathbf{2}$.


Fig. s3. Solid state UV-Vis spectra of compounds $\mathbf{1}$ and $\mathbf{2}$.


Fig. s4 the RhB photocatalytic degradation performance over compound $\mathbf{1}$.


Fig. s5. (a Time course of H 2 evolution from 50 mg of $0.1 \% \mathrm{Pt}$ loaded photocatalyst compound 1 under 300 W Xe-lamp irradiation in 100 mL of aqueous solution containing $10 \mathrm{vol} \%$ methanol solution. (b) Time course of the total H 2 evolution in 6 hours.


Fig. s6 Fig. $2 \mathrm{H}_{2}$-evolution upon Xe-lamp irradiation of 10 mg of $0.1 \% \mathrm{Pt}$ loaded PONb catalysts in $100 \mathrm{~mL} \mathrm{MeOH}-\mathrm{H}_{2} \mathrm{O}$ solution $(10 \%$ $\mathrm{v} / \mathrm{v})$.

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Scheme s1. Schematic illustration of the proposed reaction mechanism for the styrene oxidation reaction.

References:

1. I. D. Brown and D. Altermatt, Acta. Cryst. , 1985, B41, 244.
