

Supporting information

Photocatalytic hydrogen evolution over Pt-Pd dual atomic sites anchored on TiO₂ nanosheets

Yaxin Zhou^{a,b}, *Hao Qin*^{a,b}, *Sihan Fang*^{a,b}, *Yangyang Wang*^{a,b}, *Jun Li*^{a,c}, *Giuseppe Mele*^d, *Chen Wang*^{a,b,*}

a School of Chemical Engineering, Northwest University, Xi'an, Shaanxi 710069, China.

b International Science & Technology Cooperation Base for Clean Utilization of Hydrocarbon Resources, Chemical Engineering Research Center of the Ministry of Education for Advanced Use Technology of Shanbei Energy, Collaborative Innovation Center for Development of Energy and Chemical Industry in Northern Shaanxi, Northwest University, Xi'an, 710069, China.

c Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of the Ministry of Education, School of Chemistry & Materials Science, Northwest University, Xi'an, Shaanxi 710069, China

d Department of Engineering for Innovation, University of Salento, Via Arnesano, 73100 Lecce, Italy

E-mail address: wangchen@nwu.edu.cn

Synthesis of Pt SA/Vo-TiO₂ and Pd SA/Vo-TiO₂

A typical method was used to deposit single atoms on the surface of Vo-TiO₂. Dispersed 0.5g Vo-TiO₂ in 100mL deionized water and sonicated for 10 minutes. While stirring, slowly add 12.5 mL (NH₄)₂CO₃ (1M) dropwise. After that, 355 μ L of H₂PtCl₆ solution (7.2 mM) and 210 μ L of PdCl₂ solution (22.4 mM) were added dropwise to the above solution, respectively. After stirring for 5 hours, it was filtered, washed and vacuum dried at 60°C for 8 hours. The dried powder was treated at 250°C under an argon hydrogen atmosphere (the total flow is 40 mL/min, and the hydrogen to argon flow ratio is 1/9) for 2 hours. The resulting product was labeled Pt SA/Vo-TiO₂ and Pd SA/Vo-TiO₂.

Synthesis of Pt NP/TiO₂ and Pd NP/TiO₂

For comparison, the above treatment was directly performed on TiO₂ without oxygen vacancy, and the resulting product was labeled Pt NP/TiO₂ and Pd NP/TiO₂.

Table S1 ICP analysis of TiO₂, Vo-TiO₂, Pt-Pd NPs/TiO₂ and Pt-Pd SAs/Vo-TiO₂.

Catalysts	Pt (wt.%)	Pd (wt.%)
TiO ₂ NS	0	0
Vo-TiO ₂	0	0
Pt-Pd NPs/TiO ₂	0.09	0.02
Pt-Pd SAs/Vo-TiO ₂	0.09	0.02

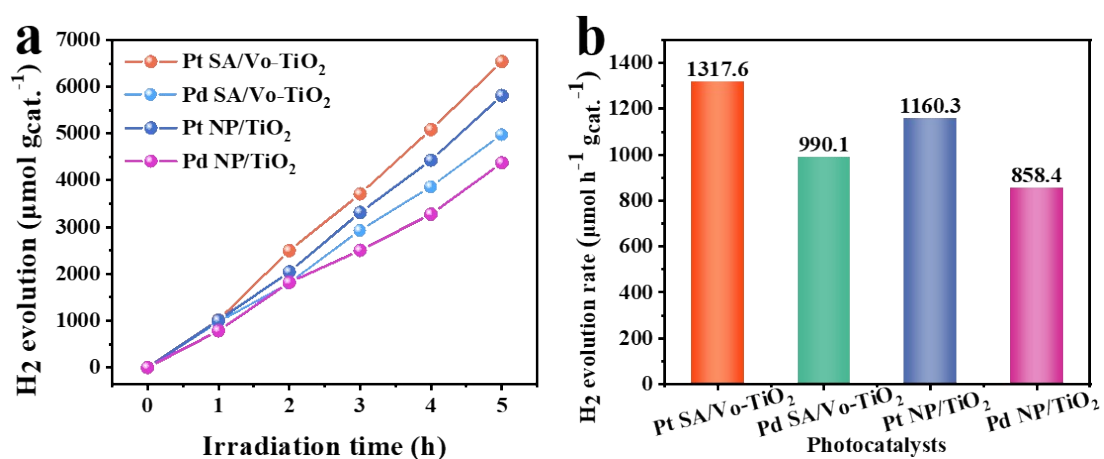


Fig. S1 (a) Photocatalytic H₂ evolution of Pt SA/Vo-TiO₂, Pd SA/Vo-TiO₂, Pt NP/TiO₂ and Pd NP/TiO₂, (b) the photocatalytic activities of all catalysts for H₂ evolution rate.

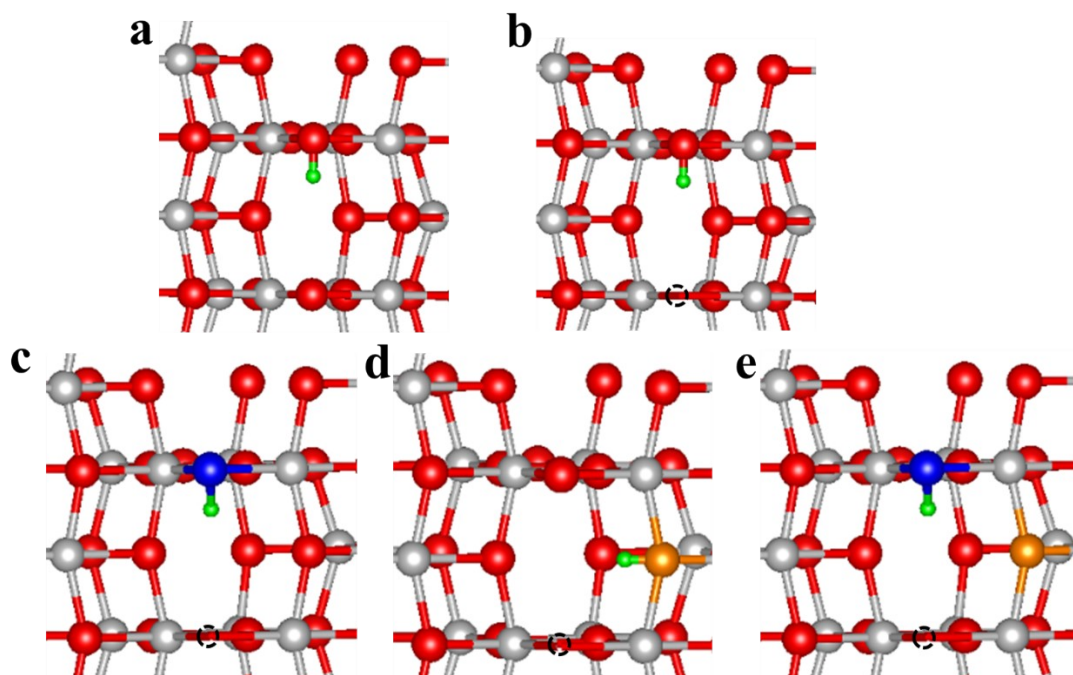


Fig. S2 Geometrical structures of H adsorption on (a) TiO_2 , (b) Vo-TiO_2 , (c) Pt SA/ Vo-TiO_2 , (d) Pd SA/ Vo-TiO_2 and (e) Pt-Pd SAs/ Vo-TiO_2 (Ti: grey, O: red, Pt: blue, Pd: orange, H: green).