Supplementary Material

Noble-metal-free $Ni_3N/g-C_3N_4$ photocatalysts with enhanced hydrogen production under visible light irradiation

Lu Chen,[a] Huijuan Huang,[a] Yuanhui Zheng,[a,b,*] Wenhao Sun,[a] Yi Zhao,[a] Paul Francis,[b,*] Xuxu Wang[a,*]

[a]State Key Laboratory of Photocatalysis on Energy and Environment, College of Chemistry, Fuzhou University, Fuzhou, Fujian, 350116, China

[b]Centre for Chemistry and Biotechnology, School of Life and Environmental Sciences, Faculty of Science, Engineering and Built Environment, Deakin University, Waurn Ponds, Victoria 3216, Australia

*yuanhui.zheng@fzu.edu.cn; paul.francis@deakin.edu.au; xwang@fzu.edu.cn

Computational Methods and Results

All calculations were performed using density functional theory （DFT）within the plane-wave pseudopotential as implemented in the VASP[1] code with a cutoff energy of 450 eV. The Perdew, Burke, and Ernzerhof (PBE) exchange-correlation functional within a generalized gradient approximation (GGA)[2] was employed. The PAW[3] method was used to describe the effect of core electrons. Gamma-centered k-point meshes of 3 × 3 × 1 were used. The atomic positions were relaxed until the force on each atom was less than 0.01 eV/Å. Using the periodic slab model and self-consistent dipole correction, the averaging electrostatic potential in the planes perpendicular to the slab normal could be obtained. We built a periodic slab with Ni_3N (111) facets, 1 × 1 surface unit cells were used. The bottom two layers are fixed, while the top two layers are relaxed during the calculation. The vacuum gap thickness was set to be 15 Å. The work function of Ni_3N (111) facets is calculated to be 5.29 eV.

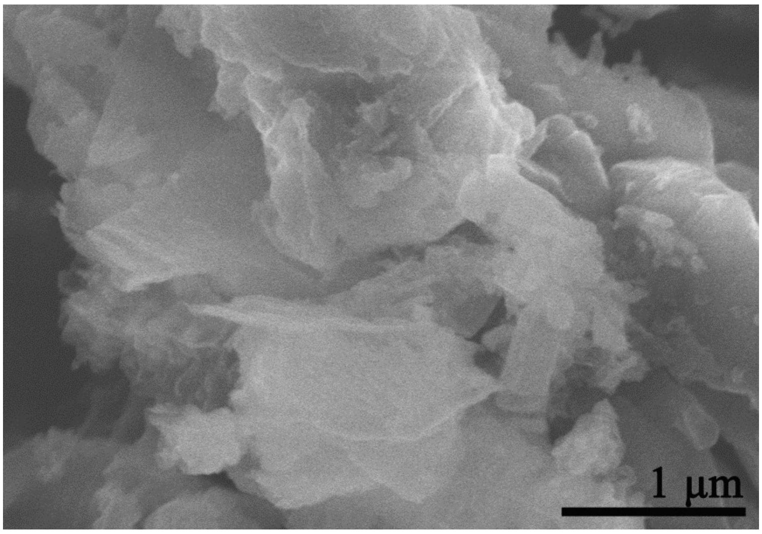

Fig. S1. SEM images of the as-prepared g-C_3N_4 sample.

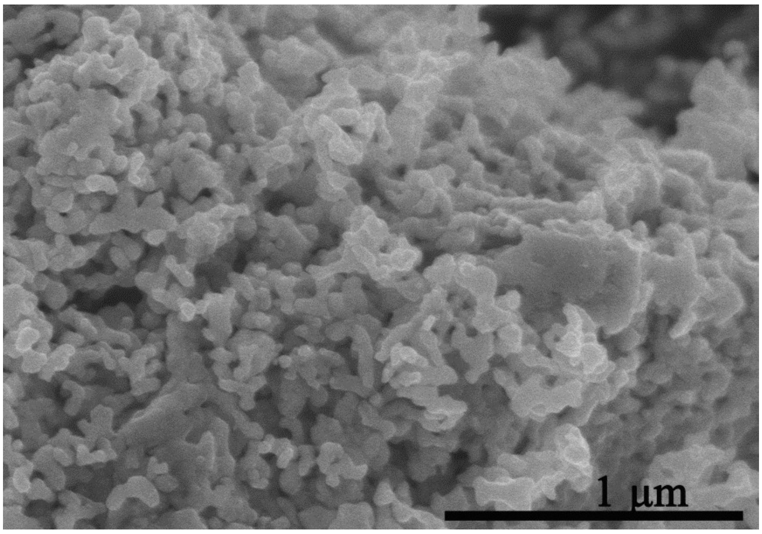

Fig. S2. SEM images of the as-prepared Ni_3N sample.

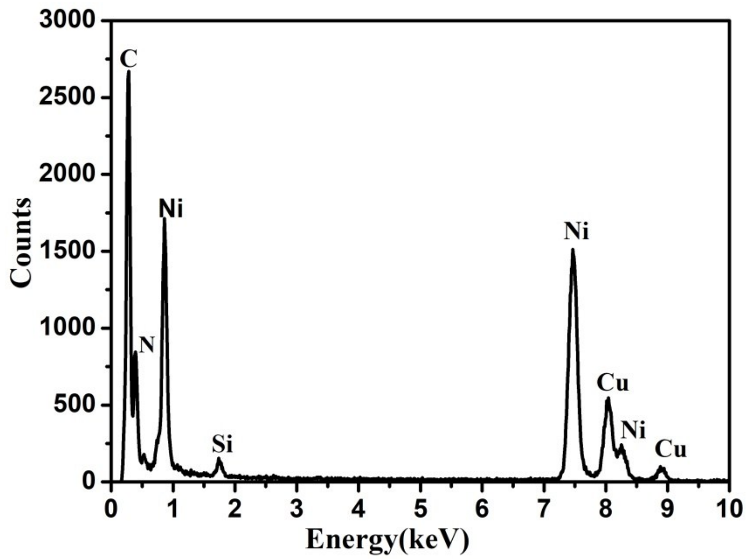

Fig. S3. Energy dispersive x-ray (EDX) spectrum of Ni_3N (3wt%)/g-C_3N_4 sample.

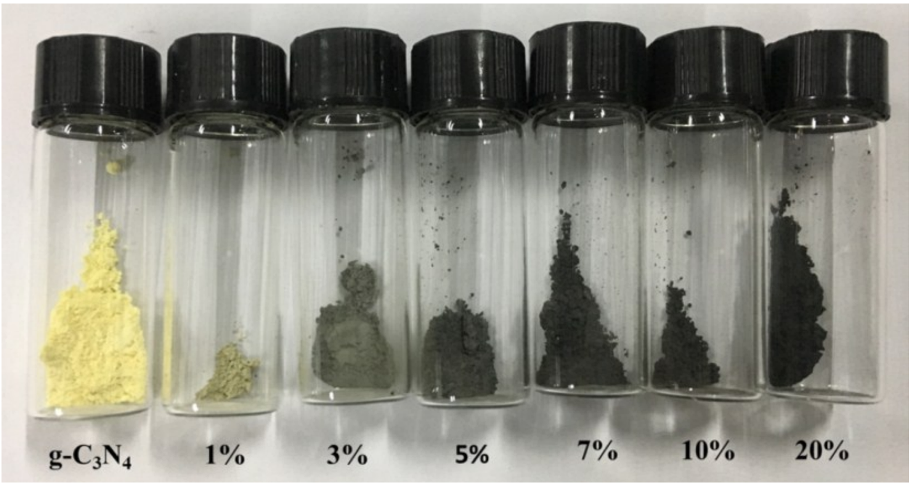

Fig. S4. Digital photographs of the as-prepared samples with different Ni_3N loading concentration.

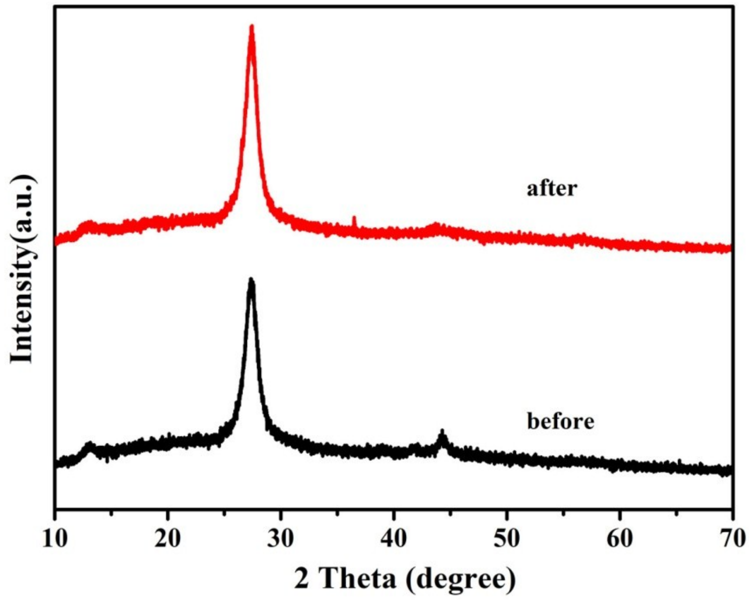

Fig. S5. XRD patterns of a 3% Ni_3N/g-C_3N_4 sample before and after H_2 evolution testing.

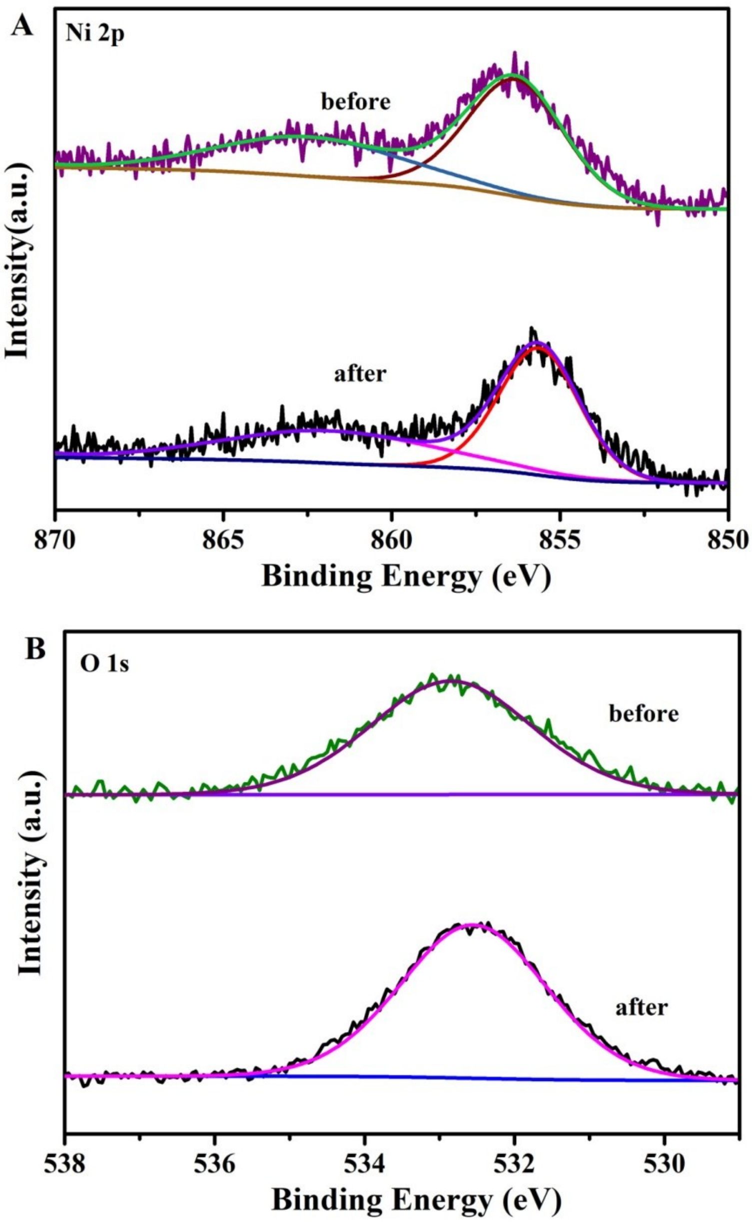

Fig.S6. XPS spectra of (a) Ni $2p_{3/2}$ and (b) O 1s of 3% $Ni_3N/g\text{-}C_3N_4$ before and after irradiation

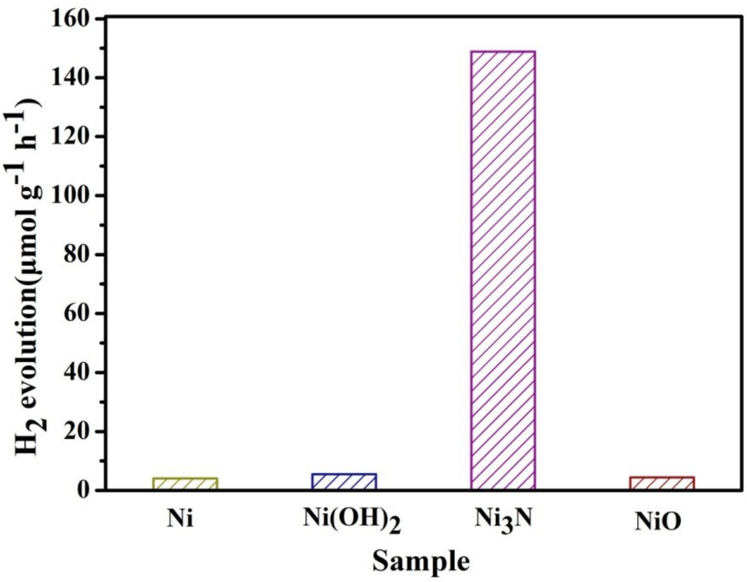

Fig.S7. Photocatalytic performance of $Ni/g\text{-}C_3N_4$, $Ni(OH)_2/g\text{-}C_3N_4$, $Ni_3N/g\text{-}C_3N_4$ and $NiO/g\text{-}C_3N_4$

References

1.Kresse, G.; Furthmuller, J. Phys. Rev. B 1996, 54, 11169-11186.
2. Perdew, J. P.; Burke, K.; Ernzerhof, M. Phys. Rev. Lett. 1996, 77, 3865-3868.
3. Blochl, P. E. Phys. Rev. B 1994, 50, 17953-17979