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Support material

Insight into enhanced photocatalytic activity mechanism of $Ag_3VO_4/CoWO_4$ p-n heterostructure under visible-light

Jie Xiong[1], Hong-Yan Zeng[1]*, Jin-Feng Peng[2]*, Sheng Xu[1], Zhuo-Lin Yang[1]

1 College of Chemical Engineering, Xiangtan University, Xiangtan, Hunan, 411105, China

2 School of Mechanical Engineering, Xiangtan University, Xiangtan, Hunan, 411105, China

*Corresponding Author:

Hong-Yan Zeng

Address: College of Chemical Engineering, Xiangtan University, Xiangtan, Hunan, 411105, China

E-mail address: hongyanzeng99@hotmail.com

Tel.: +86-0731-58298175

Jin-Feng Peng

E-mail address: pengjinfeng@xtu.edu.cn

DFT calculation

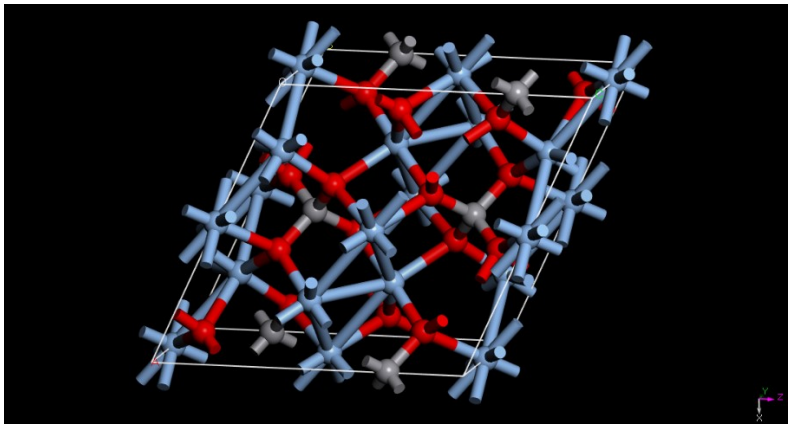
All the calculations based on DFT were carried out by using the CASTEP code. With the cutoff energy of 300 eV, the ultrasoft pseudopotentials were chosen to perform the calculation for the planewave basis set. The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) exchange correlation function was adopted for the structural optimization and self-consistent total energy calculations[1,2].

For the Ag_3VO_4 models, when performing geometric optimization, the energy cut-off is set to 300.0 eV. The maximum force exerted on the atom is 0.05 eV/Å, the maximum atomic displacement is 0.002 Å, the self-consistent convergence accuracy was set at 2×10^{-5} eV per atom, the convergence criterion for the force between atoms was 0.05 eV $Å^{-1}$. And the Monkhorst-Pack k-point grid is set to 3×3×1, and the optimized lattice parameters for Ag_3VO_4 were found to be a = b = 5.67 Å and c = 10.20 Å in good agreement with experimental values (Fig. S1) and Powder Diffraction of the Ag_3VO_4 was shown in Fig. S2. For the Ag_3VO_4 (220) surface models, the Monkhorst-Pack k-point grid is set to 1×2×1. The energy cut-off is set to 260.0 eV, the maximum force exerted on the atom is 0.05 eV/Å, the maximum atomic displacement is 0.002 Å, and the maximum energy change is 1.0×10^{-5} eV/Å.

For the $CoWO_4$ models, when performing geometric optimization, the energy cut-off is set to 300.0 eV. The maximum force exerted on the atom is 0.05 eV/Å, the maximum atomic displacement is 0.002 Å, and the maximum energy change is 1.0×10^{-5} eV/Å. The Monkhorst-Pack k-point grid is set to 3×2×2, and tthe optimized lattice parameters for $CoWO_4$ were found to be a =4.70, b = 5.77 Å and c = 5.06 Å in good agreement with experimental values (Fig. S3)

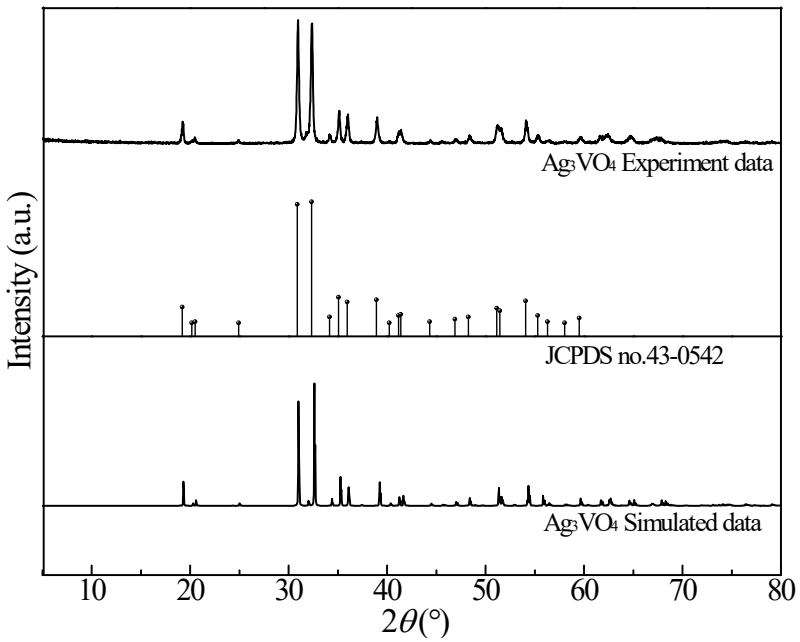
and Powder Diffraction of the $CoWO_4$ was shown in Fig. S4. For the $CoWO_4$ (-111) surface models, the Monkhorst-Pack k-point grid is set to 1×1×1. The energy cut-off is set to 260.0 eV, the maximum force exerted on the atom is 0.05 eV/Å, the maximum atomic displacement is 0.002 Å, and the maximum energy change is 1.0×10^{-5} eV/Å.

Fig. S1



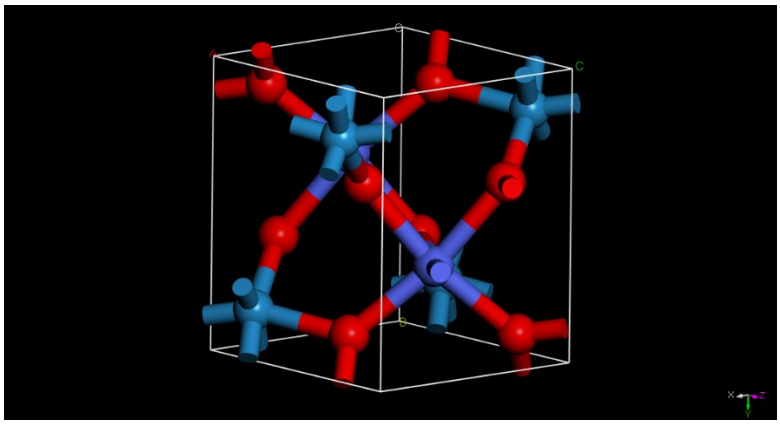
Atomic crystal structure diagram of the Ag_3VO_4

Fig. S2



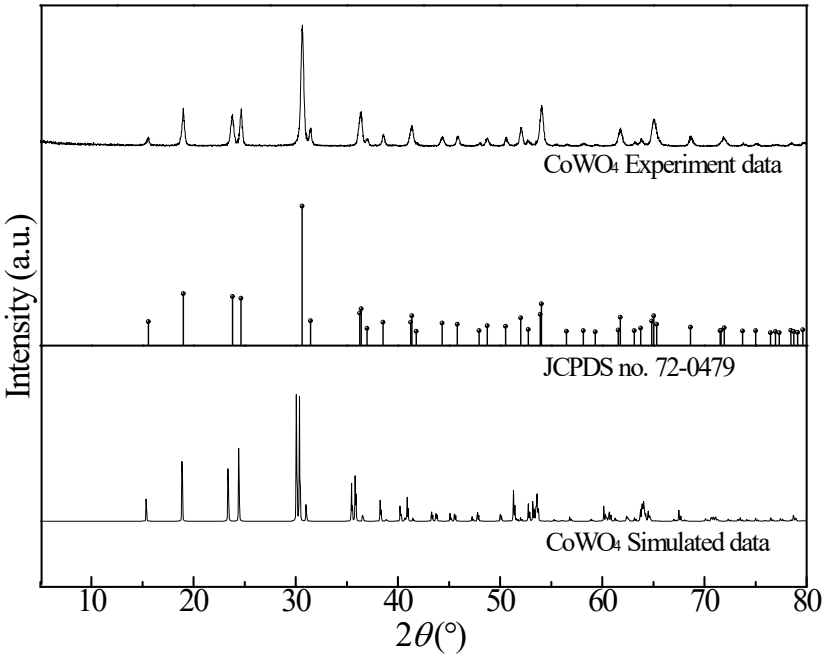
Powder Diffraction of the Ag_3VO_4

Fig. S3



Atomic crystal structure diagram of the $CoWO_4$

Fig. S4



Powder Diffraction of the $CoWO_4$

References

[1] Clark, S. J., Segall, M. D., Pickard, C. J., Hasnip, P. J., Probert, M. I., Refson, K., Payne, M. C. (2005). First principles methods using CASTEP. Z. Krist.-Cryst. Mater. 220(5-6), 567-570.

[2] Perdew, J. P., Burke, K., Ernzerhof, M. (1997). Generalized gradient approximation made simple (vol 77, pg 3865, 1996). Phys. Rev. Lett. 78(7), 1396-1396.