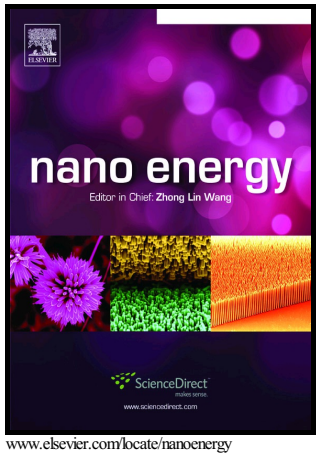

www.elsevier.com/locate/nanoenergy

Surface Step Decoration of Isolated Atom as Electron Pumping: Atomic-Level Insights into Visible-Light Hydrogen Evolution

Xin Wu, Huabin Zhang, Juncai Dong, Mei Qiu, Jintao Kong, Yongfan Zhang, Yang Li, Guilan Xu, Jian Zhang, Jinhua Ye

PII: S2211-2855(17)30812-1
DOI: https://doi.org/10.1016/j.nanoen.2017.12.039
Reference: NANOEN2420

To appear in: *Nano Energy*

Received date: 26 September 2017
Revised date: 26 November 2017
Accepted date: 23 December 2017

Cite this article as: Xin Wu, Huabin Zhang, Juncai Dong, Mei Qiu, Jintao Kong, Yongfan Zhang, Yang Li, Guilan Xu, Jian Zhang and Jinhua Ye, Surface Step Decoration of Isolated Atom as Electron Pumping: Atomic-Level Insights into Visible-Light Hydrogen Evolution, *Nano Energy,* https://doi.org/10.1016/j.nanoen.2017.12.039

Surface Step Decoration of Isolated Atom as Electron Pumping: Atomic-Level Insights into Visible-Light Hydrogen Evolution

Xin Wu,[†] Huabin Zhang,*[,‡] Juncai Dong,[§] Mei Qiu,[⊥] Jintao Kong,[†] Yongfan Zhang,[⊥] Yang Li,[†] Guilan Xu,[†] Jian Zhang,*[,†] Jinhua Ye*[,‡]

[†] *State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, China*

[‡] *International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan*

[§] *Beijing Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China*

[⊥] *College of Chemistry, Fuzhou University, Fuzhou 350108, China*

Corresponding author: Zhang.huabin@ntu.edu.sg, zhj@fjirsm.ac.cn, Jinhua.Ye@nims.go.jp

Abstract

Here we realize the decoration of isolated platinum atoms onto the surface step of CdS nanowires. The single-atom co-catalyst with high stability can realize maximum atom efficiency and significantly boost electron-hole separation efficiency in chromophore units, generating a greatly enhanced photocatalytic hydrogen evolution performance, 7.69 times as high as Pt nanoparticles do and 63.77 times higher than that of bare CdS nanowires. Directional migrations of photogenerated excitons from the conduction band of CdS to catalytic platinum centers have been witnessed by transient absorption spectroscopy, leading to the supply of long-lived electrons for highly efficient photocatalytic hydrogen evolution. Density functional theory calculations further confirm that the excellent catalytic performance is associated with positively charged platinum sites with partially vacant 5d orbitals, which change distribution of charge density and facilitate higher excited carrier density.