Copyright WILEY-VCH Verlag GmbH & Co. KGaA, 69469 Weinheim, Germany, 2017.

Small Micro

Supporting Information

for Small, DOI: 10.1002/smll.201603574

GaP/GaNP Heterojunctions for Efficient Solar-Driven Water Oxidation

Alireza Kargar, Supanee Sukrittanon, Chang Zhou, Yun Goo Ro, Xiaoqing Pan, Shadi A. Dayeh, Charles W. Tu,* and Sungho Jin*

Copyright WILEY-VCH Verlag GmbH & Co. KGaA, 69469 Weinheim, Germany, 2016.

Supporting Information

GaP/GaNP Heterojunctions for Efficient Solar-Driven Water Oxidation

Alireza Kargar, Supanee Sukrittanon, Chang Zhou, Yun Goo Ro, Xiaoqing Pan, Shadi A. Dayeh, Charles W. Tu,* and Sungho Jin*



Figure S1. Selected area electron diffraction (SAED) pattern of (a) an area of n-GaP, (c) an area including both i-GaNP and p^+ -GaP layers (TEM image of selected region is shown in (b)), and (d) i-GaNP and (e) p^+ -GaP of selected areas in (b). The combined SAED pattern (Figure S1c) is very similar to the SAED pattern of i-GaNP (Figure S1d) and p^+ -GaP (Figure S1e).



Figure S2. (a,b) HRTEM images of surface structure of n-GaP/i-GaNP/p⁺-GaP thin film substrate with the identified facets.



Figure S3. Cyclic voltammetry (CV) measurement under illumination of the TiO_2/Ni -coated n-GaP and n-GaP/i-GaNP/p⁺-GaP thin film heterojunction substrates recorded at a scan rate of 10 mV/s in 1 M KOH electrolyte.



Figure S4. Approximate energy band diagram of the TiO₂-coated (a,b) n-GaP and (c,d) n-GaP/i-GaNP/p⁺-GaP substrates at equilibrium condition and at dark, which was simulated using SCAPS (version 3.1.02) numerical simulation software. The band gap of anatase TiO₂ layer deposited by ALD was considered to be 3.2 eV.^[1,2] The electron affinity of TiO₂ (anatase and ALD deposited) was considered as ~4.3 eV.^[1,3] The doping concentration of the ALD-deposited anatase TiO₂ is in the range of 10^{17} cm⁻³ ^[4] (was considered 10^{17} in the simulation). The considered TiO₂ thickness was 20 nm based on its deposited thickness.

References

- [1] M. Perego, G. Seguini, G. Scarel, M. Fanciulli, F. Wallrapp, J. Appl. Phys. 2008, 103, 043509.
- D. O. Scanlon, C. W. Dunnill, J. Buckeridge, S. A. Shevlin, A. J. Logsdail, S. M. Woodley, C. R. A. Catlow, M. J. Powell, R. G. Palgrave, I. P. Parkin, G. W. Watson, T. W. Keal, P. Sherwood, A. Walsh, A. A. Sokol, *Nat. Mater.* 2013, *12*, 798-801.
- [3] M. Gratzel, *Nature* **2001**, *414*, 338-344.
- [4] Y. J. Hwang, A. Boukai, P. Yang, *Nano Lett.* **2009**, *9*, 410-415.