

Atomic and Electronic Structures of Graphitic Carbon Nitride/Graphene Heterostructure

Sangwoo Park^{§,1}, Taehwan Jeong^{§,1}, Jae-Hun Yang^{§,2}, Hey Yeon Park², Qinke Wu¹, Hyun Min Kang¹, Hwi Je Woo¹, Seong Jun Jung¹, Hanchul Kim³, Bong Gyu Shin⁴, Youngkuk Kim⁵, Euy Heon Hwang^{1,5,7}, Jin-Ho Choy^{*,2} and Young Jae Song^{*,1,5,6,7}

¹*SKKU Advanced Institute of Nanotechnology (SAINT), Sungkyunkwan University (SKKU), Suwon, 440-746, Korea*

²*Intelligent Nanohybrid Materials Laboratory Division of Nanoscience and Department of Chemistry, Ewha Womans University, Seoul 120-750, Korea*

³*Department of Applied Physics, Sookmyung Women's University, Seoul 140-742, Korea*

⁴*Center for Quantum Nanoscience, Institute for Basic Science (IBS), Ewha Womans University, Seoul, 03760, Republic of Korea*

⁵*Department of Physics, Sungkyunkwan University (SKKU), Suwon, 440-746, Korea*

⁶*Center for Integrated Nanostructure Physics, Institute for Basic Science (IBS), Sungkyunkwan University (SKKU), Suwon, 440-746, Korea*

⁷*Department of Nano Engineering, Sungkyunkwan University (SKKU), Suwon, 440-746, Korea*

E-mail: yjsong@skku.edu

Graphitic-carbon nitride ($g\text{-C}_3\text{N}_4$) has been proposed as a new type of catalysts due to the promising catalytic properties without precious metal. Industrial interests for sustainable and renewable energy have driven many scientists to study the unique feature of $g\text{-C}_3\text{N}_4$ as a photo-catalyst.[1,2] Here, we propose that graphene-decorated $g\text{-C}_3\text{N}_4$ can be one promising candidate for metal-free hydrogen evolution under visible light with a direct bandgap of 2.51 eV and an indirect bandgap of 1.64 eV. Band-engineered electric properties of this metal-free catalyst were confirmed by scanning tunneling microscopy, spectroscopy (STM/STS) and Kelvin probe force microscopy (KPFM) along with density functional theory (DFT) to explain the electronic structures as the photo-catalyst under visible light in atomic scale. The decoration of $g\text{-C}_3\text{N}_4$ with graphene, therefore, can provide a breakthrough for allowing water-splitting reactions under visible light efficiently without precious metal.

REFERENCES:

- [1] X. Wang, K. Maeda, A. Thomas, K. Takanabe, G. Xin, J. M. Carlsson, K. Domen, M. Antonietti, *Nature Materials* **8**, 76–80 (2009).
- [2] T. S. Miller, A. B. Jorge, T. M. Suter, A. Sella, F. Corà, P. F. McMillan, *Physical Chemistry Chemical Physics* **19**, 15613–15638 (2017).