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Design of hybrid photocatalytic materials to harness charge kinetics

With the support by the National Natural Science Foundation of China (Grant No. 21101145) and the Ministry of Science and Technology of China (Grant Nos. 2014CB848900 and 2010CB923300), Prof. Xiong Yujie's laboratory at the School of Chemistry and Materials Science, University of Science and Technology of China, together with Profs. Jiang Jun and Zhang Qun, reported new progress in the design of hybrid photocatalysts for water splitting, which was published in *Angew Chem Int Ed* (2014, 53(20): 5107(11).

The separation of photoexcited electron-hole pairs is a critical step in determining the quantum efficiency of solar-to-chemical conversion in photocatalysis, while the difficulty in capturing charge kinetics information has long been a great obstacle towards designing highly efficient photocatalysts. To unravel the underlying complicated mechanisms and achieve rational design for photocatalysis systems, Prof. Xiong's team has studied the charge kinetics by integrating controlled synthesis with theoretical simulations and ultrafast spectroscopy characterizations. Recently, when designing the surface facets of semiconductor, they discovered the surface work function, the charge transfer driven by Schottky barrier and the intrinsic charge spatial separation that synergizes two effects in a semiconductor-metal hybrid structure and substantially improves the charge separation, significantly enhancing water splitting performance. At the same intersection between synthesis, simulations and characterizations, this research team has made a series of progress in photocatalysis during the past year, including the manipulation of plasmonic hot electrons (Angew Chem Int Ed, 2014, 53(12): 3205(9), the reduction of interfacial charge recombination (Adv Mater, 2014, 26(32): 5689(95), and the specific delivery of photo-induced charges to reaction sites (Adv Mater, 2014, 26(28): 4783(8). Besides the photocatalytic applications, this designing rule for hybrid materials has also been verified as a universal methodology for such catalytic fields as the surface polarization for electrocatalytic hydrogen evolution (Angew Chem Int Ed, 2014, DOI: 10.1002/anie. 201406468). It is anticipated that this investigation methodology would be further implemented in designing catalytic materials and deeply understanding the charge kinetics in related material systems.



Figure Schematic illustrating the important role of facet selection in the Cu₂O-Pd hybrid system during water splitting.

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