Nano-Micro Conference

Abstract View Online

Electrocatalytic hydrogen evolution reaction of MX_2 and MX_2 heterostructures

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Received: 02 June 2017, Accepted: 16 June 2017, Published Online: 14 October 2017
Citation Information: Yanfeng Zhang, Nano-Micro Conference, 2017, 1, 01025 doi: 10.11605/cp.nmc2017.01025

Abstract

Advanced materials for electrocatalytic andphotoelectrochemical water splitting are central to the area of renewable energy. Recently, two dimensional layered materials of MX_2 (M: Mo, W; X:S, Se, etc.) have emerged as a new kind of catalysts for such applications. Our group have reported the direct synthesis of high-quality, domain size tunable, strictly monolayer MoS_2 flakes on commercially available Au foils by a chemical vapor deposition (CVD) method. The nano-sized triangular MoS_2 flakes on Au foils are proven to be excellent electrocatalysts for hydrogen evolution reaction (HER), featured by a rather low Tafel slope (61 mV/dec) and a relative high exchange current density (38.1 μA/cm^2). The excellent electron coupling between MoS_2 and Au foils is considered to account for the extraordinary HER activity [1]. Furthermore, via a facile all-CVD approach, we have also demonstrated the direct growth of monolayer MoS_2 on graphene (MoS_2/Gr) over Au foils [2,3]. A dramatic decrease of the bandgap from ~2.20 to ~0.30 eV was detected at the domain edge of MoS_2 within a lateral distance of ~6 nm, as evidenced by STM/STS observations. The edges of monolayer MoS_2 nano-sheets were thus served as narrow-gapquantum wires, which can greatly facilitate the electrocatalytic property of MoS_2 in HER [4]. Meanwhile, we also synthesized either MoS_2/WS_2 or WS_2/MoS_2 vertical heterostructures on Au foils by a growth-temperature-mediated, selective two-step CVD strategy. Relative enhancement or reduction in the photocatalytic activities were observed for MoS_2/WS_2 and WS_2/MoS_2 in HER under illumination, respectively. This is explained from the type-II band alignment of the MoS_2/WS_2 stack that enables effective electron-hole separation and fast electron transfer kinetics, as well as directional electron flow from electrode to catalytically active sites [5]. The abovementioned efforts are expected to establish the internal relationship between the metallic edge states of MoS_2 and its HER performances, as well as the advantage of MX_2/MX_2 vertical stacks in photocatalytic HER applications.

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