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Perspective of Transition Metal Dichalcogenide Monolayers as Catalysts in Water Electrolysis

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Two-dimensional (2D) transitional metal dichalcogenides (TMDs) have recently attracted great attention due to their intriguing physical, chemical, electronic and magnetic properties, as well as diverse applications [1-4]. A TMD monolayer is one layer derived from the layered TMD structures, which is noted as a chemical formula of MX_2 , where M is a transition metal element, and X is a chalcogen (S, Se, or Te). Within the TMD monolayer, one metal-atom sub-layer is sandwiched between two X-atom sub-layers, where M-X bonds are mainly covalent by nature. The thickness of a TMD monolayer is about 2.5 ~ 4.0 Å. Generally, after applying proper external forces to layered TMDs, it's feasible to get few-layered TMDs, and even TMD monolayer. Generally, there are mainly three fabrication methods: liquid exfoliation, lithium intercalation and chemical vapor deposition (CVD)[1]. Liquid exfoliation method is suitable for large quantity fabrication, whereas lithium intercalation method serves high yield efficiency with inducing of phase transition in MX_2 monolayers. Furthermore, CVD method is dominantly used for the fabrication of large TMD monolayers with high quality.

The easy fabrication of 2D TMDs drives the increasing investigation on their unique properties and potential applications. Tuning and control of their electronic and magnetic properties through functionalization, hydrogenation, external strain and morphology modification have been a hot topic for their diverse applications [5-11]. For example, superb flexibility of MoS_2 nanoribbons under a wide range of strain led to changes of their magnetic properties, and they can be semiconducting or metallic by controlling their different edge states [5,8] Voiry et al. found that the covalent functionalization resulted in dramatic changes in optoelectronic properties in MoS_2 nanosheets[9]. Pan found that hydrogenated VTe_2 exerts an anti-ferromagnetism to ferromagnetism transition through paramagnetic tuning point, as well as a transition from semiconducting to metal, even half-metal as the applied strain increases[10,11].

The various applications of 2D TMDs attribute to utilizing their

controllable physical and chemical properties [1,2]. Especially in facilitating hydrogen evolution reaction (HER) in electrolysis of water, TMD monolayers play a promising role of being effective electrocatalysts, even though platinum is still considered to be the archetypical catalyst for HER [12-14]. Due to the scarcity of Pt on earth, replacing Pt with cheap and abundant novel catalysts has become a very intriguing topic in both academic and industrial world concerning that hydrogen holds more expectation as a new energy source replacing fossil fuel[15-22]. Both experimental and theoretical studies have showed that 2H- MoS_2 monolayer is catalytically active for hydrogen evolution reduction (HER) ascribed to its the metallic edges, whereas its basal planes are catalytically inert. [15,16] Voiry et al. also reported that the metallic 1T- WS_2 nanosheets instead of the semiconducting 2H- WS_2 showed excellent HER performance, also which can be enhanced by applying tension[17]. A lot of work involving experiments and calculations has been investigated to maximize the efficiency of catalysts based on MoS_2 and WS_2 monolayers [18-22]. For example, Kibsgard et al. invented an atomic scale model to fabricate MoS_2 with more edges in order to enhance its water electrolysis performance [18]. Tsai and Wang et al. took much effort in predicting the improved HER catalytic efficiency by doping transitional metal atoms into both the basal plane and the edges of MoS_2 monolayer based on first principles calculation[21,22]. Most recently, Pan reported that the HER performance of VX_2 monolayers mainly depend on the choice of X atom and various hydrogen coverages, among which VS_2 has high electrolysis performance comparing with Pt at lower hydrogen coverage at its basal plane[24]. Furthermore, Qu and Pan found the HER performance of VS_2 nanoribbon edges depends on the ribbon width and configuration of the edge, narrow VS_2 nanoribbons with intact zigzag edges shows excellent catalytic performance at a wide range of hydrogen coverage based on first principles calculation [25].

Finding novel 2D TMDs as effective electrocatalyst comparative

to platinum is still challenging. Many proposed new 2D TMD based catalysts still cannot replace platinum because of either their low catalytic performance at high hydrogen coverages or the difficulties in large quantities of catalysts fabrication. New methods need to be invented to improve both conductivity and yield of TMDs monolayers. 2D TMDs are expected to be the next generation catalysts to replace platinum in water electrolysis with their controllable physical and chemical properties by methods as choice of doping, defect, functionalization, edges configurations, applying external tension, etc.

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