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Perspectives of Two-dimensional Transition Metal Dichalcogenide Monolayers

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Editorial

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The discovery of graphene, a novel two-dimensional (2D) nanostructure, has triggered an extensive study on monolayers for diverse applications in Nano devices, optoelectronics, sensors, catalysts, and energy storage because of the easy fabrication, exceptional charge transport, thermal, optical, chemical, and mechanical properties [1]. As one of important members of 2D monolayers, 2D transition metal dichalcogenides (TMDs) monolayers show a wide range of electronic, optical, mechanical, chemical, and thermal properties [2]. TMDs have a chemical formula of MX_2, where M is a transition metal element from group IV, group V, or group VI, and X is a chalcogen (S, Se, or Te). They are layered materials with weakly van der Walls interaction holding together. Each layer is a sandwich structure (X–M–X), where a M-atom layer is enclosed within two X layers and the atoms in layers are hexagonally packed [3]. Depending to stacking orders and metal atom coordination, the overall symmetry of TMD can be hexagonal or rhombohedral, and the metal atoms have octahedral or trigonal prismatic coordination.

Different from graphene, the diverse physical and chemical properties of TMDs, such as semiconductor, metal, and magnetism, can be achieved by configuring the compositions of MX_2, functionalizing, and applying external fields [4-7]. For example, 2D MoS_2 nanoribbons can be semiconducting, metallic, or magnetic by controlling its edge states and the magnetic properties of zigzag 2D $MoS2_2$ nanoribbons can be efficiently enhanced by applying strain due to their super-flexibility [5,8]. Koh et al. reported that MoS_2 can be used as mechanical valve to control molecule diffusion [4]. Recently, Pan reported that the magnetic properties of VX2 monolayers can be tubed by hydrogenation [9]. By combining hydrogenation with external tension, Shi et al. reported that magnetic properties of MoS_2 monolayer can be tuned from non-magnetism, to ferromagnetism, and further to non-magnetism with the increase of tension [6]. Most recently, Pan found that hydrogenated VX_2 monolayers transfer from anti-ferromagnetism to ferromagnetism via a turning-point of paramagnetism, and switches from semiconductor, to metal, further to half-metal as tension increases [10]. The anti-ferromagnetism with semiconducting or metallic characteristic under low tension is contributed to super-exchange or mobile-carrier enhanced super-exchange, while the ferromagnetism with half-metallic character under high tension is induced by carrier-mediated double exchange.

The chemical properties of TMD monolayers have also widely investigated, especially the catalytic activity for water electrolysis. The electrolysis of water is considered a well-known principle to produce oxygen and hydrogen gas in a sustainable fashion. The key component in electrochemical reduction of water is the catalyst for hydrogen evolution reduction (HER). Experimental and theoretical studies showed that the metallic edges of 2H-MoS_2 are responsible for its electrocatalytic activity in electrolysis of water [11,12]. Voiry et al. [13] reported that metallic 1T-WS_2 nanosheets showed better HER performance than semiconducting 2H-WS_2, which can be further improved by strain engineering. Most recently, Pan reported that the HER performances of MX_2

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monolayers depend on M, X and H-coverage and found that VS_2 is comparable to Pt for electrolysis of water at lower H-coverage and its catalytic activity can be further enhanced by improving conductivity [14].

In summary, the MX_2 monolayers and nano ribbons provide a lot of opportunities for the investigation of fundamental phenomena and their practical applications. Their versatile and tunable properties and diverse compositions make them applicable from catalyst, energy storage, sensor, and membrane to quantum devices. The literatures showed that their attractive multi-functional applications could be further achievable by controlling the doping, functionalization, external fields, edge structures, etc.

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