# 2D Materials-based Photoelectrochemical Cells: Combination of Transition Metal Dichalcogenides and Reduced Graphene Oxide for Efficient Charge Transfer

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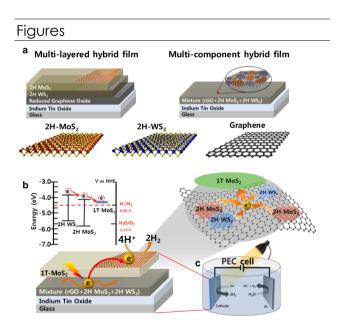
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### Abstract

Transition dichalcogenides metal (TMDs) and their hybrids with reduced graphene oxide (rGO) have attracted attention areat for use as electrocatalysts to replace Pt. However, their applications for photoelectrochemical (PEC) cells are not widely known. Herein, we report the fabrication of highly efficient photocathodes for PEC cells using only twodimensional (2D) materials, MoS<sub>2</sub>, WS<sub>2</sub> (with 1T and 2H phases) and rGO sheets. Two types of hybrid films were prepared based on various combinations of the components and optimization of the thickness; multi-layered (1T MoS<sub>2</sub>/ 2H MoS<sub>2</sub>/ 2H WS<sub>2</sub>/ rGO/ ITO) and multicomponent (1T MoS<sub>2</sub>/ (2H MoS<sub>2</sub> + 2H  $WS_2 + rGO)/ITO$  films. The hybrid films with the same component materials but different structures showed high efficiency when used as cathodes in PEC cells in terms of the current density under illumination: the increase by 60 and 67%, respectively, for the multilayered and the multi-component films. Furthermore, the roles of each component were identified. The 1T MoS<sub>2</sub> layer contributes to catalytic activity for hydrogen evolution reaction<sup>1</sup>. The hybrid of 2H MoS<sub>2</sub> and 2H WS<sub>2</sub> with different band structures facilitates more efficient carrier

transport through band proper alignment than the individual MoS<sub>2</sub> or WS<sub>2</sub> sheets<sup>2</sup>. The rGO sheets act as conductive interconnecting components prevent the to recombination of electrons and holes. Finally, the optimized hybrid film (1T  $MoS_2/$  (2H  $MoS_2$  + 2H  $WS_2$  + rGO)/ rGO/ ITO), based on above roles of each component, showed highly efficient PEC performance. This study points out that the performance of PECs consisting of 2D materials is affected by the combination of 2D materials and the structure of the photoelectrode.



**Figure 1:** (a) Schematic illustration of the two types of rGO/TMD based hybrid films. (b) Charge transfer processes for the hydrogen evolution reaction and the (c) measurement system inside a PEC cell. The inset in (b) shows the energy level diagrams of 2H MoS<sub>2</sub> and 2H WS<sub>2</sub>.

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