Low-Workfunction Metal Doping for Making WSe_2 Photovoltaic Devices

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Layered transition metal dichalcogenides (TMDCs) are potentially implemented for making new photo-response devices, such as ultra-thin-film photovoltaic (PV) cells and ultra-broadband photodetectors. To build such photo-response devices, built-in potentials need to be formed in TMDC-based photoactive layers for separating photo-generated electron-hole (e-h) pairs. Currently, the research community lacks suitable techniques for generating permanently stable built-in potentials in pristine TMDCs layers. Conventionally, the built-in potentials are formed in semiconductors through doping processes. The conventional doping methods for bulky semiconductors, such as ion implantation and thermal diffusion, can cause detrimental damage to 2D materials.[1] Utilizing additional electrodes to generate electrostatic doping effects, Pospischil *et al.* demonstrated WSe_2 photo-diodes.[2] However, such a device structure is not suitable for practical PV applications. Furchi *et al.* fabricated heterojunction photo-diodes based on vertically stacked MoS_2/WSe_2 layers, and such devices have exhibited sizable photovoltaic responses. However, we still lack a nanofabrication method cable of producing such heterostructures over large areas.[3] Recently, our team developed metal-film-induced surface-charge-transfer (SCT) method capable of forming potentials in WSe_2 layers and generating photovoltaic responses[4].

In this work, we extended the SCT principle to create large built-in potentials in p-type TMDCs (*e.g.*, WSe_2) using low-workfunction metal (*e.g.*, Mg) coating. Specially, we developed a coating process able to result in a high-quality Mg/WSe_2 interface that is the key to obtain a large potential barrier in WSe_2 layers for separating photo-generated e-h pairs. Using Mg-coated WSe_2 PV devices, we have achieved high photo conversion efficiencies (PCEs) up to 10% under 532 nm laser illumination.

Fig. 1 shows the optical micrograph of a representative Mg-coated multilayer WSe_2 PV device, which consists of a vertically stacked ITO/5 nm Mg/multilayer WSe_2/Au structure. The most critical step to fabricate such devices is the coating of high-quality, uniform, and continuous Mg film on top of WSe_2 layers. We have systematically studied the dependence of the Mg film quality on the deposition condition parameters. We found that the resultant Mg film quality and device performance is highly sensitive to the initial deposition chamber vacuum. Through optimizing the deposition condition, we have achieved ITO/Mg/WSe_2/Au devices with PCEs up to 7.1% under 532 nm laser illumination (Fig. 2a). In addition, we also created ITO/WSe_2/Mg/Au devices with PCEs up to 10% (Fig. 2b). More details about the formation of high-quality Mg/WSe_2 interfaces and the fabrication of WSe_2 PV devices will be presented in the final presentation.

This work has advanced the processing knowledge for modulating electronic and optoelectronic states in emerging layered semiconductors and enabling practical photo-response device applications.

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[2]A. Pospischil, M. M. Furchi & T. Mueller, Nature nanotechnology, 9(4), 257-261, 2014.
[3]M. M. Furchi, A. Pospischil, F. Libisch, J. Burgdörfer & T. Mueller, Nano letters, 14(8), 4785-4791, 2014
[4]S. Wi, M. Chen, D. Li, H. Nam, E. Meyhofer, X. Liang Applied Physics Letter, 107, 062102, 2015

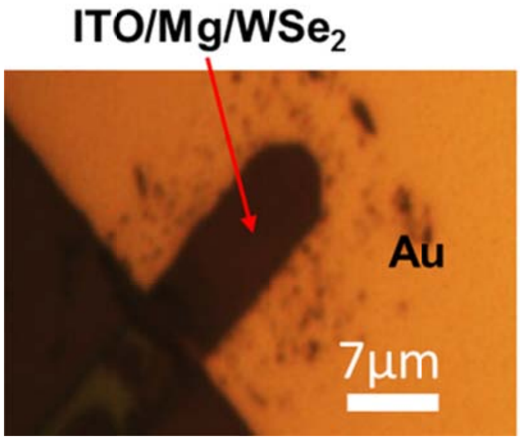

Fig. 1 Optical micrograph of a representative ITO/Mg/WSe_2/Au PV device.

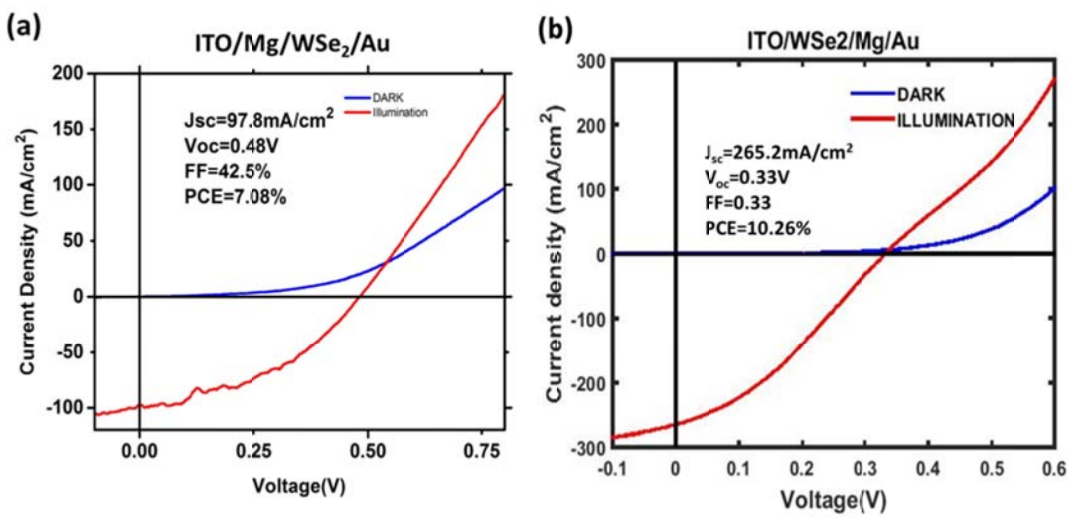

Fig. 2 Photovoltaic characteristics measured from (a) an exemplary ITO/Mg/WSe_2/Au PV device, and (b) an exemplary ITO/WSe_2/Mg/Au PV device.