Visible-light driven water oxidation from Large Area 2D MoS_2/WS_2 Heterojunctions

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Solar electrochemical energy conversion devices including dye-sensitized solar cells and photoelectrochemical (PEC) water splitting systems are crucial tools to mitigate the future environmental impact from fossil fuel consumption. In PEC systems, composed of a cathode performing the hydrogen evolution reaction (HER), and a photoanode where oxygen is evolved, the water-oxidation reaction requires significantly more energy (four electron-hole pairs compared to two), and is the bottleneck to energy efficient devices (Gratzel, 2001).

2D layered materials, including transition metal dichalcogenides, are of great interest for opto-electronic devices due to their layer dependant electronic properties and visible light absorption. Recent theoretical work has shown that both MoS_2 and WS_2 at mono-layer have the potential to function as a photoanode for water oxidation (Kang *et al.* 2013). Experimentally, we have recently realized this in the form of thin films of chemically exfoliated MoS_2/WS_2 heterojunctions for water oxidation, which demonstrate a synergistic effect beyond either individual components performance (Pesci *et al.* 2017). This effect arises from efficient charge transfer between the two van der Waals stacked components leading to electron-hole separation and increased reaction time at the surface (Pesci *et al.* 2017). Whilst these heterostructures are excellent as proof-of-concept devices, the photocurrents and incident photon-to-current efficiency values are quite low compared to state-of-the-art materials.

Here, we present a high crystal quality MoS_2/WS_2 heterostructures grown by chemical vapour deposition for salt water oxidation (Sherrell, *et al*. 2019). These heterostructures demonstrate photocurrents densities up to 0.8 mA/cm^2 (at 1-sun, +0.7V vs Ag/AgCl) and IPCE peaking at 1.6% in 3.5% NaCl. This performance is superior to both liquid phase processed heterostructures for water oxidation and WSe_2 for photo catalytic hydrogen evolution. These heterostructures can be grown over a cm^2 area with a high electrochemically active surface area (100 m^2/g) and can be transferred onto a variety of flexible substrates for device specific requirements, paving the way for the use of 2D crystal heterostructures in water splitting devices and provide a viable option for the energetically challenging water oxidation reaction.

References

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