A VAN DER WAALS HETEROJUNCTION BASED ON MONOLAYERS OF MoS_2 AND WSe_2 FOR SOLAR WATER SPLITTING

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The production of clean, sustainable and economical hydrogen is one of the major challenges to face the depletion of fossil fuels and their detrimental environmental impacts. Among others, solar water splitting (SWS) has been widely studied as a promising technology for generating carbon-free hydrogen. Here, we propose a monolithic SWS system based on a *Z-Scheme* van der Waals heterojunction (vdWH) using monolayers of transition metal dichalcogenides (TMD) as active core materials (Fig 1). This structure provides the bias required for electrolysis ($V_{oc} > 2$ V) while maximising the absorption of solar energy[1] with small bandgaps. MoS_2 and WSe_2 are *a priori* chosen for the anode and cathode respectively because of their electrochemical[2, 3, 4, 5] and optical[6, 7] properties. Two distinct regions make up the active core. The first is a MoS_2/hBN/WSe_2 heterojunction (Fig 2). Hexagonal boron nitride (hBN) is used to isolate the two TMDs[8]. The electrons (holes) photogenerated in WSe_2 (MoS_2) are consumed by the hydrogen (oxygen) evolution reaction. In the second region, hBN is removed to ensure the recombination of the extra carriers (i.e. holes in WSe_2 and electrons in MoS_2). Membranes of mesoporous transparent metal oxides support the heterojunction and enable water to reach the active part. To understand the behaviour of our system, we developed a multiphysics model that computes the solar-to-hydrogen (STH) efficiency of the system. In this model, we use *ab initio* calculation to determine the optical porperties of the active materials and we implement the detailed balance method and the Butler-Volmer kinetics to simulate the photoelectrochemical response. Under realistic operating conditions, the system achieves an STH efficiency greater than 15%. Since our system is wireless and requires simple manufacturing processes (exfoliation), this result is remarkable.

References

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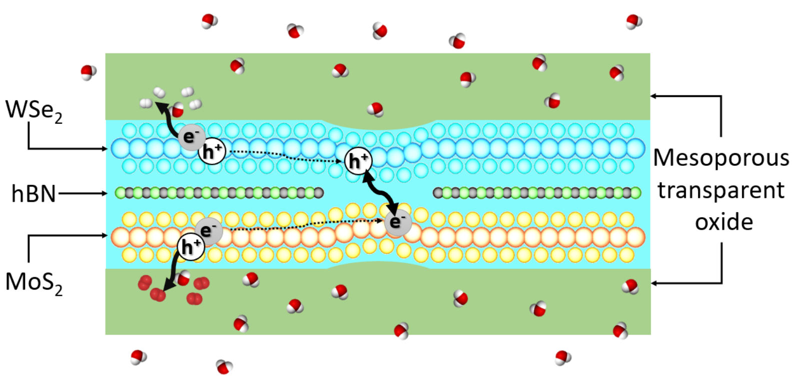

Figure 1: Schematic representation of the SWS system. The active core is based on a MoS_2/hBN/WSe_2 vdWH and a MoS_2/WSe_2 vdWH. The former enables the carrier generation and the electrochemical reactions and the latter ensures the extra carriers recombination. A transparent mesoporous oxide supports and protects the active core.

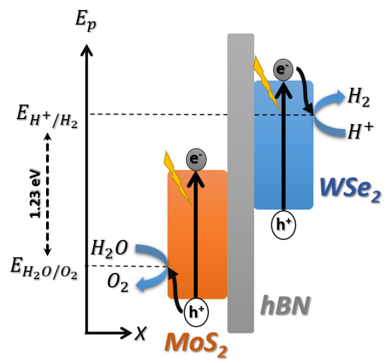

Figure 2: Sketch of the band diagram in the first region where MoS_2 and WSe_2 are isolated by hBN. E_{H^+/H_2} and E_{H_2O/O_2} are respectively the reaction potentials of the reduction of H^+ in H_2 and of the oxidation of H_2O in O_2.

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