Ultra-thin van der Waals heterostructure: how thin can a diode be?

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With the advent of atomically thin van der Waals materials, it is now possible to combine p and n doped 2D semiconductors to realize p-n junctions at their ultimate thickness. [1-3] Due to the lack of a depletion width in atomically thin van der Waals materials, however they are conceptually different compared to conventional diode. [4] Here, we demonstrated strong rectification behaviour for a p-n junction made of bilayer n-type MoS_2 and ultrathin (10 nm) p-type GaSe with a rectification ratio of 10^4. The threshold voltage is determined to be 0.57 V. The I – V characteristics under illumination using below band gap excitation reveals a marked photovoltaic effect suggesting efficient exciton dissociation due to the presence of an electric field at the interface. The below band gap excitation also suggests the presence of accessible states in the forbidden gap of MoS_2. To validate our experimental observations we also performed DFT calculations on such heterostructure. Our theoretical findings indicate that the electronic band structure of bilayer MoS_2 is modified by the interaction with GaSe. This interaction creates accessible states in the forbidden gap of MoS_2 and may explain the below band gap excitation and the rectification behaviour of the p-n junction.

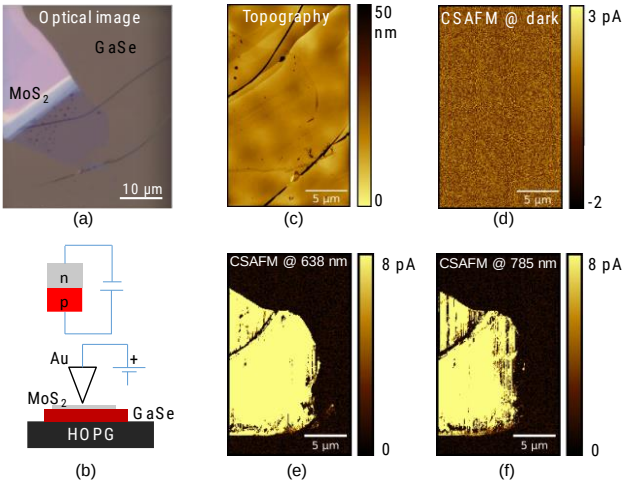

Figure: GaSe/MoS_2 p-n junction. (a) optical image of the heterostructure, (b) schematic of the device and experiment, (c) AFM topography of the diode, and (d) – (f) CSAFM images of the diode in the dark and illumination

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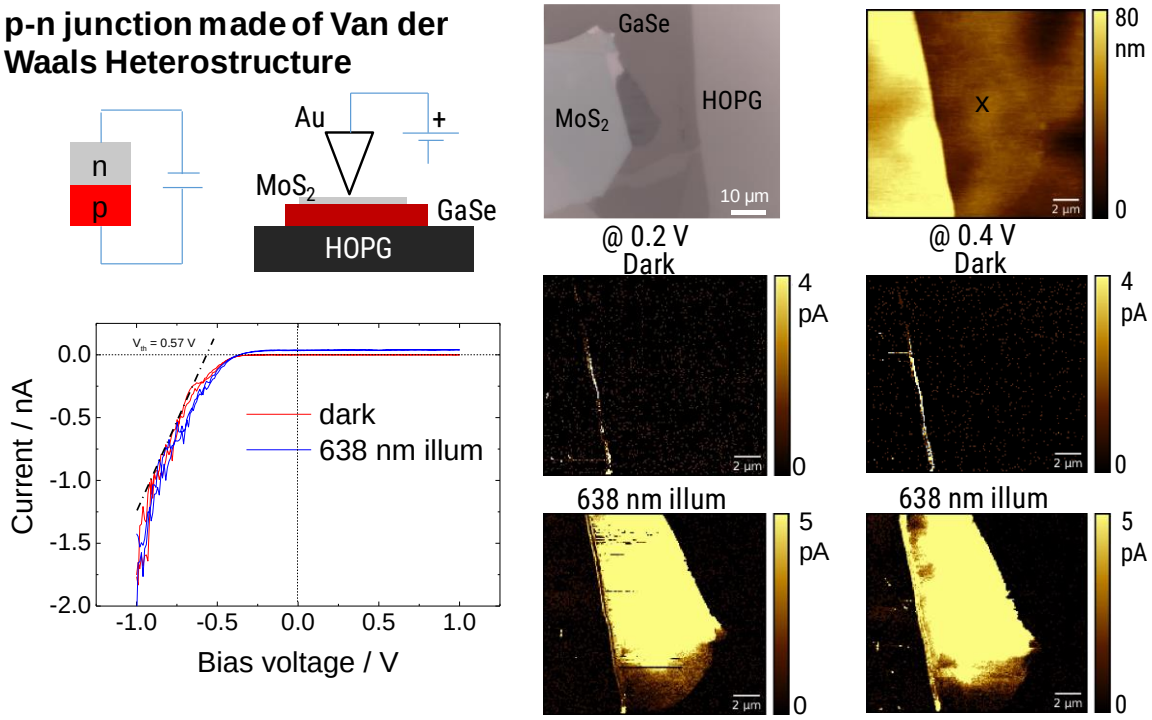

Figure: Demonstration of the formation of p-n junction in ultra-thin van der Waals vertical heterostructure. The schematic of the device and the experimental configuration (top left). Optical image of the heterostructure and the AFM topography (top right). The I – V curves in the dark and illumination taken on the cross mark shown in topography (bottom left). CSAFM images in the dark and under illumination at different voltages (bottom right).

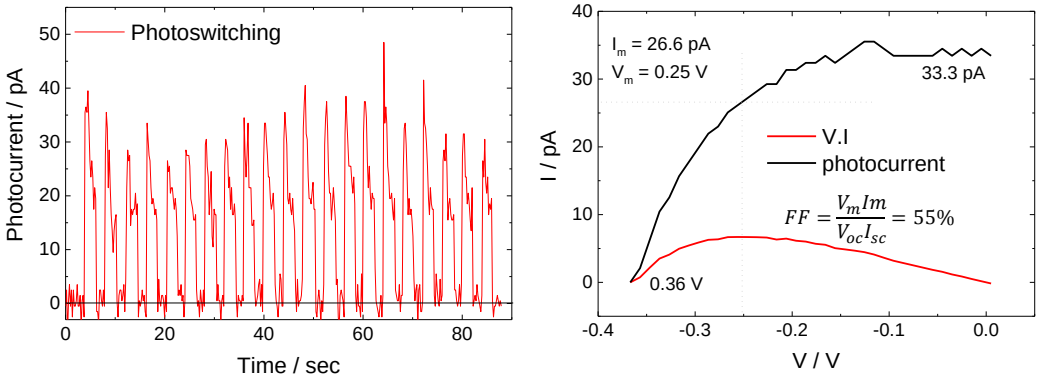

Figure: Demonstration of photodetector and photovoltaic application. Photoswitching experiment of the diode was performed at 0 V under 638 nm illumination. The fill factor of the diode was determined to be 0.55 under 638 nm illumination.