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Enhanced Optoelectronic Performances of the 2D Semiconductor Transition Metal Dichalcogenide Heterojunction via Introducing Monolithically-Band-Engineered Charge Transport Layer

To realize the high-performance optoelectronic devices based on 2D semiconductor transition metal dichalcogenides (TMDs), it is inevitably required to promote charge transport at the interface between active semiconductors and electrodes as well as enhancing absorption of incident light and dissociation of photogenerated excitons. Nevertheless, the effective strategies to improve charge collection in various TMD heterojunctions have rarely been explored, while substantial research efforts have been made to improve light absorption and exciton dissociation processes in such devices. Here, we report a novel approach to improve optoelectronic device performances of the 2D WSe_2-MoS_2 *p-n* heterojunction by employing the monolithically-band-engineered charge transport layer. In the proposed device architecture, the atomically thin WO_x layer that acts as a hole extraction layer was monolithically formed by layer-by-layer oxidation of the WSe_2. Significant enhancements of photoresponse characteristics in terms of photocurrent, photovoltage and power conversion efficiency were consistently observed in the monolithic-oxide-inserted heterojunction devices compared with those of the simple WSe_2-MoS_2 heterojunctions. In particular, the power conversion efficiency is increased by about an order of magnitudes, from 0.6 to 5.1 %, while the response time is maintained at 2~3 ms although WO_x is used as an interlayer. This is because the introduction of the oxide layer leads to effective charge transport and collection at the hole contact due to the Schottky barrier lowering at the interface, which was also supported by first principle calculations.