Interlayer Excitons Engineering in Transition Metal Dichalcogenides Heterobilayer

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Abstract. Our study is aimed to showcase the feasibility of manipulating the optical characteristicsof transition metal dichalcogenide heterobilayers, particularly when one ofthe constituent layers adopts a ternary structure. The focal point of our investigationlies in the intriguing class of structures known as type II band alignment. This manipulation bears crucial implications for enhancing charge separation efficiency, as optically excited electrons and holes undergo relaxation into distinct material layers. In the realm of binary–ternary heterostructure systems, we have unveiled an exciting avenue for extending the energy range and tailoring emission energies, surpassing the capabilities of their binary counterparts. Remarkably, even when some binary–ternary heterostructures exhibit nearly identical optical gaps, their band offsets diverge. This discrepancy leads to charge transfer between the monolayers following optical excitation,revealing a nuanced interplay within these systems. Our findings underscore the significance of ternary transition metal dichalcogenide alloys in fine-tuning band offsets, thereby introducing a novel design parameter for tailoring optoelectronic devices to specific applications. This insight not only advances our understanding of the unique properties within these materials but also paves the way for the development of highly customizable and application-specific optoelectronic devices.

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