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Tight binding approach to study electronic properties of MoS_2/WS_2 heterostructure NAMITA NARENDRA, KI WOOK KIM, North Carolina State Univeristy — The heterostructure interface of MoS_2/WS_2 is being increasingly studied in recent years for its electronic and optical properties. The ability to tune properties of few-layer transition metal dichalcogenides (TMDs) by strain engineering provides a significant incentive to further explore these material interfaces. It has been shown that misorientation in bulk MoS_2 and WS_2 can also alter the electronic properties. Tight binding allows us to calculate the transport properties of MoS_2/WS_2 interface for all the angles of misorientation, unlike the computationally limited first principles approach. In this work, the tight binding parameters for the bulk are extracted from first principles and the heterostructure model is verified. A detailed study of variation of electronic properties of MoS_2/WS_2 interface with respect to addition of strain and number of layers of MoS_2 and WS_2 is carried out. The extension of tight binding model to misoriented MoS_2/WS_2 interface is demonstrated.

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