Electrical Control of Interlayer Physics in Type-II TMD Heterostructures

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We describe the electronic and topological properties of $MoSe_2/WSe_2$ heterostructure using a combination of density functional theory (DFT) and tight-binding (TB) approximation. We start with determining the electronic structure of $MoSe_2/WSe_2$ from first principles, using the PBE parametrization of the GGA for the exchange-correlation potentials and including atomistic spin-orbit interaction. We obtain type-II band alignment and conduction band minima at Q points in agreement with previous works [1,2]. We include the analysis of Kohn-Sham wavefunctions allowing to describe the leading layer, spin and orbital contribution for a given band and given point in the reciprocal space, as well as to capture the interplay between two types of valleys present in the conduction band, i.e. K and Q. Following our previous work on monolayers we construct the *ab initio*-based TB model [3] for $MoSe_2/WSe_2$ heterostructure, which allows us to understand orbital contributions to Bloch states and will enable further studies of both twisted transition metal dichalcogenide (TMD) heterostructures and TMD-based multi-million atom nanostructures. To validate the model, we perform the analysis of topological properties of the system manifested in the Berry curvature. Finally, we perform a study of the effect of electric field on the interlayer properties of the $MoSe_2/WSe_2$ heterostructure towards the construction of gate-tunable spin-valley qubits [4] in TMD heterostructures.

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