Excitons in Transition Metal Dichalcogenide Heterostructures

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Single layers of transition metal dichalcogenides (TMDs) MX_2 (M = Mo, W; X = S, Se, Te) are novel semiconductor research platforms enabling exploration of many fundamental physical phenomena. These include, e. g., low energy massive Dirac fermions, valley degrees of freedom which allow for selective excitation with circularly polarized light and strong electron-electron interactions leading to excitons with binding energy ~500 meV [1], robust charged exciton states [2,3] and broken symmetry valley- and spin-polarized phases [4]. TMDs are also the basic "blocks" to the construction of van der Waals heterostructures [5]. Such systems, built from atomically thin layers of MX_2 crystals, enable the formation of excitons composed of electrons and "holes" in distinct layers producing long-lived interlayer excitons with very strong binding energies [6,7] and interlayer many body complexes [8]. It is also possible to farther advance means of manipulation of properties of TMD van der Waals heterostructures with mutual twisting of layers [9].

In the following work the electronic and excitonic properties of TMD heterostructure $MoSe_2$ / WSe_2 will be described using a combination of density functional theory, tight-binding approximation and Bethe-Salpeter equation. We start with determining exciton fine structure due to type-II spin-split band arrangement, considering both A/B, spin bright/dark and intra-/inter- layer exciton series. In next step we study properties of electron and hole Bloch wavefunctions in tight-binding approximation, especially Berry curvature and its effect on the excitonic spectrum renormalization and topological splitting of the *2p*-bound exciton states.

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