Electronic effects in wrinkled 2D transition metal dichalcogenides

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Abstract

Strain engineering is an established method employed in the synthesis of 2D materials to tune their electronic properties. Wrinkling is a method of conveying complex strain to 2D materials, in contrast to the usual in-plane strain fields. Many researchers have already confirmed that this type of non-uniform strain can lead to fascinating physical phenomena such as the funneling of excitons. However, the large size of the system hindered the theoretical study of the wrinkling effects in 2D materials. We have investigated the wrinkling of monolayers and [hetero]bilayers of transition metal dichalcogenides utilizing density functional theory. WSe_2 mono- and bilayers in addition to heterobilayers of WSe_2-$MoSe_2$ are studied. Espescially in monolayers we showed that a splitting in momentum direction occurs that we have associated with the spin-orbit coupling and the symmetry breaking present in the system. Moreover, we observed the localization of band extrema on different sections of the structure which shows the origin of the localization of excitons on different layers and different sections of the heterostructure.