Electronic effects in wrinkled 2D transition metal dichalcogenides

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Abstract

Strain engineering is an established method of property tuning in 2D materials [1]. Inhomogeneous strain field, such as found in wrinkles, can be applied to 2D materials in a controlled way as was done for example in the work of Schweikart *et al.* [2]. Although wrinkles are ubiquitous in 2D materials, the difficulties in modeling them hindered thorough studies of these systems. Here, we investigate the influence of wrinkling on the electronic structure of 2D transition metal dichalcogenide monolayers of WSe_2 and $MoSe_2$. Using Density Functional Theory, we show that wrinkling can be utilised to adjust the size and type of the bandgap of these semiconducting systems (*i.e.*, direct *vs.* indirect). Moreover, nanotubes can be used to gain insight into these inhomogeneously strained system and we discuss differences that arise due to the different boundary conditions. Additionally, we show that taking spin-orbit coupling into account is crucial in the modeling of these systems due to the inherently broken symmetries; it can lead to exotic phenomena such as a large Rashba-like splitting [3] of the valence band at the Γ point.

References

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Figures

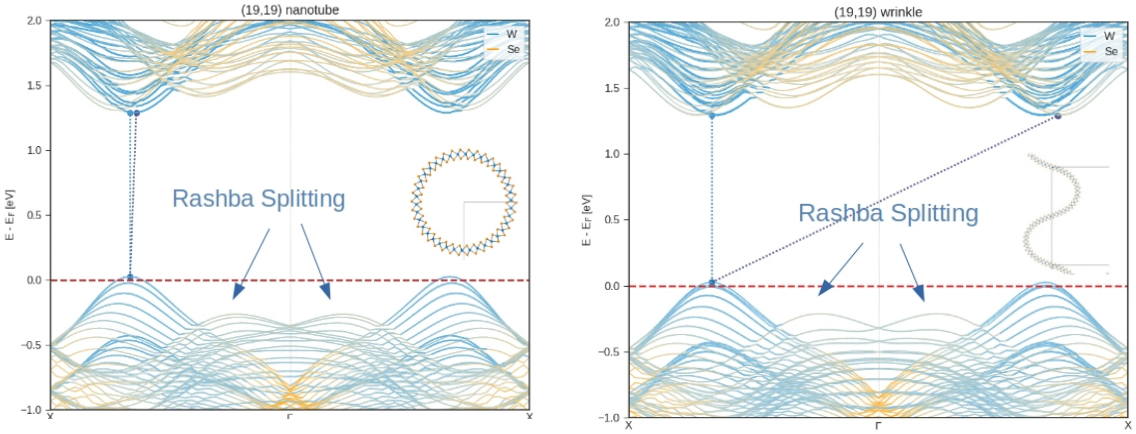

Figure 1: electronic structure of the nanotube and wrinkles of (19,19) WSe_2 , appearance of momentum direction spin-orbit coupling splitting is also shown on the figures.