Spin-orbit induced splitting in presence of non-uniform strain in 2D materials

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Abstract
Strain is omnipresent in 2D materials whether due to preparation methods or as a part of the post processing steps to obtain some special tailored properties. While the uniform strain is thoroughly studied and even data is present in public databases [1, 2], the knowledge of the effect of non-uniform strain in 2D materials is scarce. Many challenges are ahead to grasp the physics and chemistry in non-uniformly strained structures. Here, we want to investigate if 2D wrinkled structures, where non-uniform strain with different direction and magnitude is present, can be modeled as nanotubes. Moreover, Density Fuctional theory (DFT) was utilized in order to gain information about the changes in the electronic structure. Investigating WSe_2 and MoS_2 as prototypical 2D materials we found that spin-orbit coupling plays a crucial role in determining the properties especially of the valence band. Interestingly, we observed Rashba type splitting [3] which is a consequence of the symmetry breaking and is associated to the charge redistribution due to strain in these structures.

References

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Figures

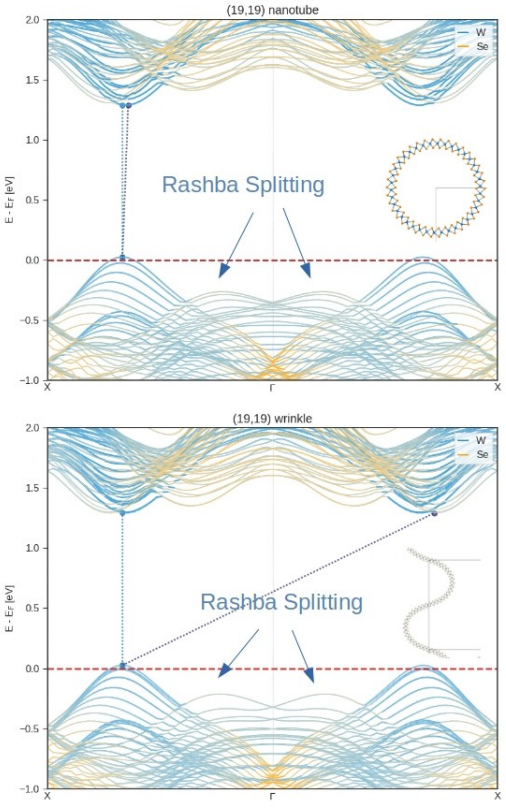

Figure 1: (right) electronic structure of the nanotube and wrinkles of (19,19) WSe_2 , appearance of momentum direction spin-orbit coupling splitting is also shown on the figures.

Figure 2: (below) relaxed structure of wrinkled monolayer of the WSe_2