Energetics and electronic properties of WS_2 nanoscroll

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Transition metal dichalcogenides (TMDs) are representative two-dimensional (2D) materials that consist of a transition metal layer sandwiched between two chalcogen layers with a thickness of three atoms. This unique atomic structure endows TMDs with remarkable physical properties, such as high carrier mobility and tunable electronic structures by the constituent atom species. These characteristics make TMDs highly attractive for various applications, such as electronics, optoelectronics, and energy storage devices. In addition to their planar conformation, recent experiments demonstrated that TMDs can also form one-dimensional (1D) conformations, such as nanoribbons, nanotubes, and nanoscrolls, which highly enhance the carrier mobility [1] and induce unusual electronic properties owing to the confinement effects. Among these 1D conformations, nanoscrolls are expected to exhibit unique physical properties ascribed to the combination of the confinement effects and the inter-shell interactions. Therefore, in this work, we investigated the energetics and electronic properties of WS_2 nanoscrolls with different scrolled conformations using the density functional theory.

The stability of the WS_2 nanoscrolls strongly depends on their innermost radius and number of shells. We also demonstrated that the local electronic structure of WS_2 nanoscroll is sensitive to the atomic position along the scroll and their conformations: The band edges of W atoms in the inner shell are deeper than those in the outer shells, which indicates that the WS_2 nanoscrolls possess type II band edge alignments, even though it has homogeneous structure [Fig.1]. This unique band edge misalignment is ascribed to the curvature effects of these shells.

Reference

[1] X. Cui, et al *Nat. Commun.* **9**, 1301 (2018)

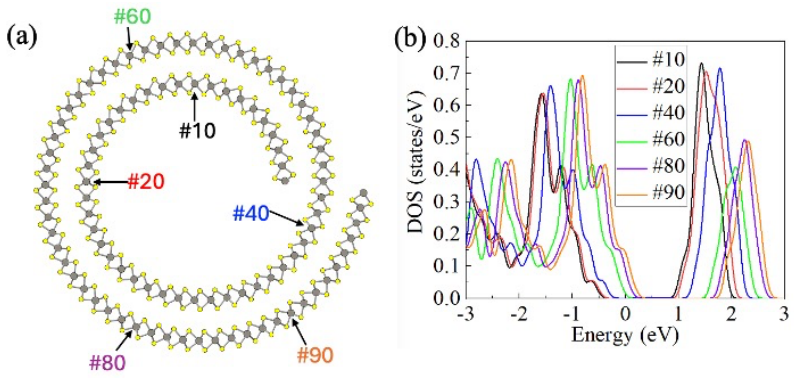

Fig. 1 (a) Geometric structure of WS_2 nanoscroll with the number of some W atoms. (b) Projected density of states of W atoms of the WS_2 nanoscroll.