Energetics and electronic properties of NbS_2 nanoscrolls

Yanlin Gao
Mina Maruyama, Susumu Okada
Department of Physics, University of Tsukuba, Tsukuba 305-8571, Japan
ylgao@comas-tsukuba.jp

Transition metal dichalcogenides (TMDs) are layered materials where a transition metal layer is sandwiched by chalcogen atom layers. They exhibit tunable electronic structures that depend on the constituent elements. TMDs can form various one-dimensional (1D) nanostructures, such as nanoribbons, nanotubes, and nanoscrolls, by applying appropriate boundary conditions. Ever since the experimental synthesis of the TMD nanoscroll, nanoscrolls have attracted much attention due to their unique morphologies [1]. TMD Nanoscrolls are expected to exhibit unique physical properties due to their self-interactions between their shells and continuously varying curvature. For instance, semiconducting WSSe nanoscroll is reported to be more stable than its flat counterparts due to van der Waals (vdW) interactions between its adjacent shells [2]. Moreover, they are semiconductors with a type-II band edge alignment along the scroll, despite their uniform composition [2,3]. Motivated by these results, we focus on the metallic NbS_2, and investigate the energetics and electronic properties of NbS_2 nanoscrolls with 22.7 nm wide NbS_2 ribbon consisting of 80 Nb atom rows using density functional theory (Figure 1).

Our results show that the structural stability of NbS_2 nanoscroll strongly depends on its conformation, corresponding to different innermost radii. NbS_2 nanoscroll has an energy minimum when the innermost radius is 1.5 nm. This stability arises from a balance between the van der Waals (vdW) interaction energy gain and the curvature-induced energy cost. NbS_2 nanoscrolls are metals, irrespective of conformations, with a large density of states at the Fermi level on all Nb atoms. Interestingly, the projective density of states is insensitive to the relative position of Nb in the scroll, and the peak position remains consistent throughout, owing to the strong electronic screening effect of the metallic nature.

References

[1] M. Kaneda, et al. ACS Nano, **18** (2024) 2772.
[2] Y. Gao, et al. Phys. Rev. B, **110** (2024) 035414.
[3] Y. Gao, et al. ACS Appl. Electron. Mater. **7** (2025) 5861.

Figures

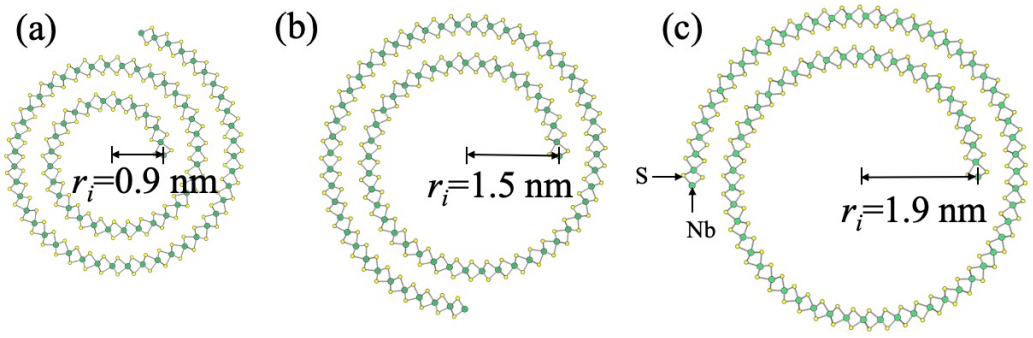

Figure 1: (a) Geometric structure NbS_2 nanoscroll with different conformation corresponding to different innermost radius.