Energetics and electronic property of Janus WSSe nanoscroll

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Janus transition metal dichalcogenides (TMDs) are in-plane heterostructures of TMDs where different chalcogen layers sandwich the transition metal layer. This structural asymmetry causes the dipole moment across its layer, causing unique electronic properties. The structural asymmetry also causes unique morphologies: Janus TMDs can possess scrolled confirmation as their ground state to gain the interlayer interaction and release the strain in their planar conformation [1-3]. Although Janus TMD nanoscrolls have been synthesized experimentally, the comprehensive knowledge about their energetics and electronic structures is still unclear. Therefore, in this work, we studied the energetics and electronic structures of Janus WSSe nanoscroll in terms of their innermost radii and the number of shells using the density functional theory. Here, we considered Janus WSSe nanoscrolls by rolling up a WSSe nanoribbon with W-terminated zigzag edges and a width of 3.3 nm containing 100 W lines.

Our calculations revealed that The WSSe nanoscrolls are more stable than the corresponding WSSe nanoribbon since the van der Walls interaction between adjacent shells and the strain relaxation by the scrolling. The most stable nanoscroll considered in this work has an innermost radius of 2.5 nm [Fig.1]. The electronic structure of Janus WSSe nanoscrolls is sensitive to their conformations. This leads to a unique local electronic structure along the scroll: WSSe nanoscrolls are semiconductors exhibiting a band bending along the scroll. This band bending results in a type II band edge alignment between the inner and outer shells, which is ascribed to the radial dipole moment induced by curvature and asymmetric chalcogen arrangement across the shell.

References

[1] M. Kaneda et al. ACS Nano,18, (2024) 2772.
[2] Y. Gao and S. Okada, Appl. Phys. Express 16, (2023) 075004.
[3] Y. Gao and S. Okada, Phys. Rev. B 110, (2024) 035414.

Figures

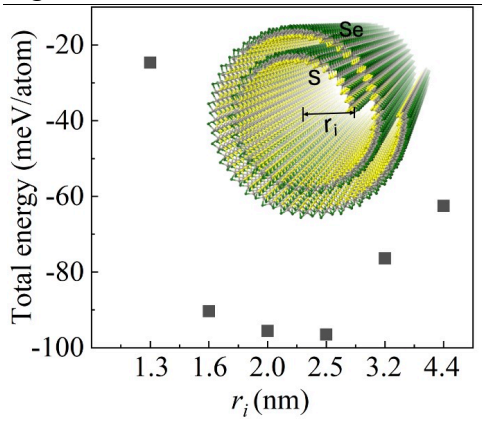

Figure 1: Total energy per atom of Janus WSSe nanoscrolls relative to the corresponding isolated flat WSSe nanoribbon.