

Energetics and morphologies of transition-metal dichalcogenide nanoscrolls

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Atomic-layer materials can form scrolled morphology known as nanoscrolls [1,2], in which the continuously varying curvature from the innermost to the outermost shells, as well as inter-shell interactions and edge effects, are decisive in determining their physical properties. Janus WSSe nanoscrolls exhibit remarkable stability and a unique electronic structure along their circumference [3]. Although the energetics and electronic properties of nanoscrolls with small diameters have been investigated, little is known about nanoscrolls with large diameters and multiple inter-shell stackings. Thus, this work aims to investigate the energetics and geometries of transition-metal dichalcogenide (TMD) nanoscrolls, using a continuous elastic model combined with inter-shell van der Waals interactions, with all parameters determined by density functional theory (DFT) [4].

Our calculations demonstrated that for short rolled lengths, strain and van der Waals effects compete to determine the nanoscroll geometry, whereas for long rolled lengths, van der Waals effects dominate. For Janus TMDs with short rolled length, the curvature induced by intrinsic strain and van der Waals interactions cooperatively leads to bistable morphologies, characterized by scroll and arch conformations. Therefore, Janus nanoscrolls could serve as building blocks for nanoscale mechanically switchable devices.

References

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Figures

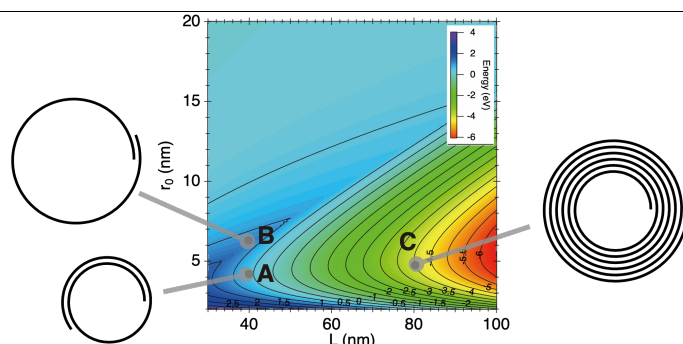


Figure 1: Total energy of WS₂ nanoscrolls as functions of its innermost shell radius and unscrolled length.