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Structural and Electronic properties of a bismuth nanowire encapsulated inside a boron nitride nanotube[1] CHI-HSUAN LEE, CHIH-KAI YANG, Graduate Institute of Applied Physics, National Chengchi University, Taipei, Taiwan, ROC — The structural and electronic properties of a bismuth nanowire (BiNW) encapulated inside the boron nitride nanotube (BNNT) are investigated by first principles calculation. The results show that they depend both on the configuration of BiNW and the diameter of the BNNT. The interaction between the two constituents induces hybridization of energy bands from each subsystem, causing unexpected variation of dispersion and splitting of energy bands near the Fermi level. The role of spin-orbit interaction is especially decisive in the later outcome. It enhances the stability of the hybrid structure and produces more band-edge states. These results should be observable with the tool of scanning tunneling spectroscopy.

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