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Band unfolding scheme for one-dimensional semiconductor nanowires SUNGHYUN KIM, KEE JOO CHANG, Dept. Physics, Korea Advanced Institute of Science and Technology — First-principles density functional calculations have been widely used to investigate the electronic structure of a variety of materials. Recently, one-dimensional nanostructures such as nanowires have received much attention because of their unique electronic properties and their building blocks of nanoscale devices. Due to quantum confinement and zone folding effects, semiconductor nanowires exhibit a complex subband structure different from those of their bulk counterparts. Using a band unfolding method, one can extract the hidden translational symmetry and compare directly the unfolded band structure with experiments such as angle resolved photoemission spectroscopy measurements. In one-dimensional systems embedded in vacuum, since confined modes exist, correspondence between the supercell and primitive reciprocal spaces is not well defined compared with perfect bulk systems. In this work, we propose a scheme for unfolding the band structure of semiconductor nanowires, in which a localized basis set is used for the band unfolding. The nanowire wave functions are described in terms of Bloch waves along the periodic wire axis and confined standing waves across the wire. For Si nanowires, we find that the unfolded band structure well recovers the hidden dispersion of bulk Si, verifying our scheme, and discuss the usefulness.

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