Spatial charge confinement in core-shell nanowire heterostructures

A. Nduwimana, R. N. Musin, A. H. Smith, and X. Q. Wang

Department of Physics and Center for Theoretical Studies of Physical Systems, ***Clark Atlanta University****, 223 James P. Brawley Drive, S.W., Atlanta, Georgia 30314*

We have employed first principles density functional theory to study the quantum confined states due to band offset in the core-shell and core-multishell structured Si/Ge and GaN/GaP nanowires. The calculation results are in agreement with experimental observations on the charge accumulation in the Ge or GaP region. The band offset effects are analyzed based on the subband charge density distributions. The band offset is found to be dependent upon the size and composition of the nanowire heterostructures. The first-principles calculation results are compared with predictions from an effective-mass model with the band-offset induced potential barrier for clarifying the symmetry of the quantum confined states.