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First-principles study of orbital-dependent quantum confinement in Si/Ge nanowire superlattices MIN-KOOK KIM, HYOUNG JOON CHOI, Yonsei University — We study electronic structures of H-passivated Si/Ge nanowire superlattices (NWSLs) oriented along [110] direction, using an *ab-initio* pseudopotential density-functional method with the local density approximation. Obtained electronic structures of the Si/Ge NWSLs show both dispersive and non-dispersive bands in conduction and valence bands due to band-selective quantum confinement: the highest valence band and the lowest conduction band are not confined in either the Si- or Ge-nanowire segment but they are extended throughout the whole NWSLs, while there exist non-dispersive bands confined in either Si- or Ge-nanowire segment below the top of the valence band and above the bottom of the conduction band. This feature originates from strong orbital-dependence of quantum confinement of electronic states, making conventional band-offset diagrams for superlattices invalid in Si/Ge NWSLs. Effects of atomic geometries on the confinement are studied with different diameters and superlattice periodicities. This work was supported by NRF of Korea (Grant Nos. 2009-0081204 and 2011-0018306). Computational resources have been provided by KISTI Supercomputing Center (Project No. KSC-2011-C3-05).

Min-Kook Kim
Yonsei University

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