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First-Principles Study of Ultrathin Single-Walled Nanotube-Based Single-Electron Transistor for Fast-Switching Applications

© Sweta Parashar

Government College, Vijaypur, District Sheopur (M.P.),
476332 India

E-mail: parasharsweta1@gmail.com

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This work presents modeling and functioning of nanotube island single-electron transistor (SET), through first-principles approach based on density functional theory and non-equilibrium Green's function. Ultrathin single-walled carbon (C), boron nitride (BN), and silicon carbide (SiC) nanotubes in armchair (3,3) and zigzag (5,0) structures have been adopted as island in the SET model. The nanotube (NT) islands are weakly coupled to gold metal electrode, explained by sequential transport phenomenon. Present study evaluates ionization energies, electron affinities, and additional energies for all the considered NTs in both isolated and SET environment, which are further analyzed by plotting total energies and Coulomb blockade diagrams. Also, various types of dielectric material and their thickness have been investigated, owing to measuring the stability of charge as well as dependence of conductance on gate and source–drain voltage. Observed results show noticeably enhanced conductance for ultrathin single-walled C, BN, and SiC zigzag NTs than that of their corresponding armchair NTs in the SET systems, demonstrating their potential for fast-switching device applications.

Keywords: single-electron transistor (SET), first-principles, nanotubes (NTs), Coulomb blockade.