Lee, Iljeong, “Multi-band Quantum Transport in a Si Nanowire”

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We present the effect of bulk Si contacts on Si nanowire transport properties and local density of states using a non-equilibrium Green’s function formalism. Using nearest-neighbor sp3d5s* empirical tight binding, a realistic Si nanowire electronic structure was calculated. Using the Si nanowire Hamiltonian from the tight-binding method, we solved the Green’s function equations for nanowire surface states and bulk Si surface states. The retarded and advanced Green’s functions were calculated using a recursive algorithm for effective calculation of the inverse matrix. From knowledge of the retarded and advanced Green’s functions, we can easily calculate the local density of states and transport properties of the free-standing Si nanowire. We also calculated the band offset arising from contact between the Si nanowire and bulk Si. Finally, we studied the effect of the bulk Si contact on the transport properties of the Si nanowire and on its local density of states using the self-energy technique.