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Atomistic study of heavy doping in Si nanowires[1] MAHESH NEUPANE, University of California, Riverside, CA 92506, RAJIB RAHMAN, Sandia National Laboratories, Albuquerque, NM 87185, USA, ROGER LAKE, University of California, Riverside, CA 92506 —
Dopant atoms are becoming increasingly important in the nanoscaled field-effect transistors (FET) because of their tendency to influence device parameters such as sub-threshold current-voltage characteristics and gate-to-channel electrostatic coupling. Achieving high doping concentrations is essential for the realization of Si nanowire FET where low resistance contacts or tunnel junctions and narrow depletion widths are needed. In an effort to understand the dopants effect on these devices as a function of scaling parameters, we use self-consistent field (SCF) tight-binding (TB) method as implemented in NEMO3D to obtain an accurate quantitative description of the band structure, confinement geometries and valley-orbit interaction from a full band-structure technique as a function of dopant location, concentration and applied electrical field. Our method solves the Poisson equation iteratively coupled with the atomistic TB Hamiltonian for charge self-consistency to provide an accurate description of the electrostatics. Our simulations show how the band structure of the nanowire is affected by the presence of few impurities.

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