High-resolution O(N) DFT method and its application to large-scale nanowire simulations

JEAN-LUC FATTEBERT, SEBASTIEN HAMEL, Lawrence Livermore National Laboratory, GIULIA GALLI, UC Davis — Using a real-space finite difference discretization and orbitals localization techniques, accurate O(N) Density Functional Theory calculations of systems made of thousands of atoms are now possible [1]. Using that methodology, we have investigated the static dielectric properties of silicon nanorods for diameters as large as 5 nm. We used a finite electric field method with non-periodic boundary conditions to calculate the dielectric response of the system, extending a previous study [2] to larger nanowires.


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