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Large-scale quantum transport calculations for electronic devices with over ten thousand atoms WENCHANG LU, YAN LU, ZHONGCAN XIAO, MIRO HODAK, EMIL BRIGGS, JERRY BERNHOLC, North Carolina State University — The non-equilibrium Greens function method (NEGF) has been implemented in our massively parallel DFT software, the real space multigrid (RMG) code suite. Our implementation employs multi-level parallelization strategies and fully utilizes both multi-core CPUs and GPU accelerators. Since the cost of the calculations increases dramatically with the number of orbitals, an optimal basis set is crucial for including a large number of atoms in the active device part of the simulations. In our implementation, the localized orbitals are separately optimized for each principal layer of the device region, in order to obtain an accurate and optimal basis set. As a large example, we calculated the transmission characteristics of a Si nanowire p-n junction. The nanowire is along (110) direction in order to minimize the number dangling bonds that are saturated by H atoms. Its diameter is 3 nm. The length of 24 nm is necessary because of the long-range screening length in Si. Our calculations clearly show the I-V characteristics of a diode, i.e., the current increases exponentially with forward bias and is near zero with backward bias. Other examples will also be presented, including three-terminal transistors and large sensor structures.

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