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Ab initio simulation and design of graphene-based transistors at the atomic scale WENCHANG LU, JERRY BERNHOLC, North Carolina State University, Raleigh, NC 27695 — Two-dimensional materials, such as graphene and molybdenum disulfide, have attracted much attention because of their unique properties. Graphene's high mobility make it a very promising material for next generation electronics, but its zero band gap is a big hurdle for digital transistors. However, graphene nanoribbons can exhibit band gaps due to quantum confinement, and their electronic properties differ depending on the structures of their edges. Based on the real space multigrid method and the non-equilibrium Green functions technique for multi-probe systems, we have developed massively parallel DFT-based software to calculate quantum transport properties with several thousands atoms. We present results for transport properties of graphene-based transistors with different atomic structures and study the effects of nanoribbon length, width and gate structure.

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