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Order(N) Parallel Tight Binding Molecular Dynamics: Applications to Carbon Nanotubes

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Abstract

Due to their novel mechanical and electronic properties, carbon nanotubes are perceived as the critical components for next generation nanoelectronic devices. Based on their chirality, single wall nanotubes exhibit metallic to insulating behavior. The conductivity of the tubes may also change due to the presence of defects (pentagonal, heptagonal or impurities) and radial deformations, as well as tensile/compressive uniaxial and torsional deformations. Using our recently developed $O(N)$ parallel tight binding program, we study the influence of defects, uniaxial tensile and compressive and torsional deformations on (10, 10) armchair nanotubes. Conventional tight binding solves the Schrödinger equation through diagonalization which leads to $O(N^3)$ behavior in cost, N being the number of atoms. In order to study the electronic properties of realistic size carbon nanotubes we have implemented a parallel, $O(N)$-scaling empirical tight binding molecular dynamics (TBMD) algorithm based on divide and conquer approach. We will also report on the performance characteristics of our $O(N)$ parallel TBMD program.

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