Building and Deploying Community Nanotechnology Software Tools on nanoHUB.org – Non-Equilibrium Green's Function Simulations of the Impact of Atomic Defects on the Performance of Carbon Nanotube Transistors. NEOPHYTOS NEOPHYTOU, SHAIKH AHMED, DIEGO KIENLE, MARK LUNDSTROM, GERHARD KLIMECK, Network for Computational Nanotechnology, Purdue University, W. Lafayette, IN 47907 — The Network for Computational Nanotechnology (NCN) is a multi-university, NSF-funded initiative with a mission to lead in research, education, and outreach deploying a unique web-based infrastructure (http://nanoHUB.org) to serve the nation's National Nanotechnology Initiative. Around 30 research codes/community tools are available and all the NCN services are free of charge. One such community tool is the CNT-FET simulator based on NEGF techniques and the Finite-Element-Method (FEM) to treat three-dimensional (3D) electrostatics. We are able to simulate electronic transport in experimentally demonstrated 3D CNT devices with atomistic potential and charge resolution. Currently, we are investigating the effects of atomistic defects in the CNT devices such as vacancies and charged impurities.

Gerhard Klimeck
Network for Computational Nanotechnology, Purdue University,
W. Lafayette, IN 47907

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