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Quantum transport and nanoplasmonics with carbon nanorings - using HPC in computational nanoscience

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Central theme of this talk is the theoretical study of toroidal carbon nanostructures as a new form of metamaterial. The interference of ring-generated electromagnetic radiation in a regular array of nanorings driven by an incoming polarized wave front may lead to fascinating new optoelectronics applications. The tight-binding method is used to model charge transport in a carbon nanotorus: All transport observables can be derived from the Green's function of the device region in a non-equilibrium Green's function algorithm. We have calculated density-of-states D(E) and transmissivities T(E) between two metallic leads under a small voltage bias. Electron-phonon coupling is included for low-energy phonon modes of armchair and zigzag nanorings with atomic displacements determined by a collaborator's finite-element based code. A numerically fast and stable algorithm has been developed via parallel linear algebra matrix routines (PETSc) with MPI parallelism to reach significant speed-up. Production runs are planned on the NSF XSEDE network. This project was supported in parts by a 2010 NSF TeraGrid Fellowship and the Sunshine State Education and Research Computing Alliance (SSERCA). Two summer students were supported as 2010 and 2011 NCSI/Shodor Petascale Computing undergraduate interns.

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