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Quantum transport in carbon nanorings for metamaterials applications[1]

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Central theme of this theoretical study is quantum transport on carbon nanoring surfaces under microwave illumination and the transmission of electromagnetic energy across a two-dimensional array of properly aligned toroidal carbon nanotubes for metamaterials applications. In a classical description, electromagnetically driven electronic surface currents in the rings will themselves generate in multipole radiation to interfere with an incoming polarized wave front, which may lead to new optical response characteristics created e.g. by the chiral features of the underlying mesoscopic structures. Possible applications ranging from quantum computing to new energy harvesting technologies could be envisioned. At these mesoscopic scales however a proper quantum mechanical treatment of these coherent electronic oscillations in form of *surface plasmon-polaritons (SPPs)* that travel along the toroidal surfaces is necessary. The main effects of SPPs in charge transport can be described in a simplified Hubbard model that allows a generalization of single-electron tightbinding transport calculations in a non-equilibrium Green's function formalism. An existing Fortran code is being expanded to include these quantum many-body effects by calculating the transport Green's function G_F using highly optimized, parallel matrix inversion routines in an object-oriented C++ code with the ScaLAPACK library on NSF *TeraGrid* resources (TACC). Multiparticle quantum effects can thus be treated accurately and quickly for realistic nanoring device sizes of few 10,000 carbon atoms or more. The influence of different torus dimensions and relative alignments may be studied on how electromagnetic energy is stored and transmitted across the metamaterial. Additionally, in a collaboration with the Georgia Institute of Technology the influence of electron-phonon coupling on transport for low-energy vibrational modes is investigated, crucial for understanding true nanodevice performance when including dissipation. This project was partially supported as a summer research project under the 2010 NCSI/Shodor Petascale Computing Undergraduate Summer Internship and the 2010 NSF TeraGrid *Pathways* Summer Faculty Fellowship Program.

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