Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Computational Design of Optoelectronic and Spintronic Devices in Graphene Nanoribbon Heterojunctions AVINASH PRAKASH, ELIF ERTEKIN, University of Illinois — Graphene is well known to possess outstanding electronic and structural properties. The potential of two-dimensional materials in creating next-generation optoelectronic computing systems has been exhibited both computationally and experimentally. In this contribution, we use first-principles total energy electronic structure methods to develop design principles for optoelectronic devices, such as resonant tunneling diodes and double heterostructure lasers, in nanostructured graphene. A density functional theory approach utilizing non-equilibrium Green's functions and the Landauer-Büttiker formalism for ballistic transport provides the spin-polarized transmission spectrum and I-V characteristics of the devices. These calculations can quantify the effects of nanoribbon topology on the device characteristics. We report negative differential resistance and spin filtering effects that can be engineered in novel logic circuits based on resonant tunneling. Our results provide the impetus to fabricate optoelectronic and spintronic devices from monomer organic molecules via bottom-up chemical synthesis methods. We elucidate the applicability of graphene nanoribbons in optoelectronic molecular computing.

Elif Ertekin
Univ of Illinois - Urbana

Date submitted: 15 Nov 2013

Electronic form version 1.4