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Quantum interference controlled graphene nanoribbon/molecule junctions: First-principles modeling of multiterminal nanoelectronic devices KAMAL K. SAHA, BRANISLAV K. NIKOLIC, Dept. of Physics and Astronomy, University of Delaware, Newark, DE 19716 — The recent fabrication of graphene nanoribbons (GNRs) has opened unforeseen avenues for carbon nanoelectronics by providing new type of semiconducting channel for field-effect transistors (FETs) or interconnect electrodes for molecular devices. GNRs can resolve one of the key challenges for molecular electronics—a well-defined molecule-electrode contact with good transparency and reproducibility–through a unified π-bonded network across GNR and conjugated molecule. However, very little is known about such devices, which is partly due to the lack of first-principles tools that can handle atomistic and electronic structure of the device while taking into account more than two electrodes at finite bias voltage. Here we propose a *three-terminal* device composed of [18]annulene ring-like organic molecule attached to two GNRs with zigzag edges in a configuration that ensures destructive quantum interference of electron paths around the ring and minuscule transmission at the Fermi level as the off-state. The third electrode is then coupled to the device to switch it into the on-state. Using our recently developed nonequilibrium Green function formalism combined with the density functional theory for multiterminal devices, we demonstrate FET-like operation of this heterojunction.

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