Graphene Nanoribbon(GNR) based Nanoelectronics for Interconnect Applications and Logic Devices using First Principles Calculations[1] YU ZHOU, SUBBALAKSHMI SREEKALA, YIMING ZHANG, PHILIP SHEMELLA, Rensselaer Polytechnic Institute, PULICKEL AJAYAN, Rice University, SAROJ NAYAK, Rensselaer Polytechnic Institute, RPI TEAM — We have studied electronic structures of graphene ribbon based nanoelectronics using first principles density functional techniques for interconnect applications as well as for logic devices. The conductance behaviors of them are computed based on Nonequilibrium Green's Function. For example, we have calculated the energy gap and I-V curve of Schottyky diode built by connecting two zig-zag GNRs with different passivations. All new configurations will show nonlinear I-V behavior and explicit step feature is observed in the I-V plot as well. There is also a small charge transfer at the junction area for this new configuration which is more like a traditional diode, which leads to different phenomena during the negative biasing.

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