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Transport Properties of p-n Junctions Formed in Boron/Nitrogen Doped Carbon Nanotubes and Graphene Nanoribbons[1] MAHMOUD HAMMOURI, IGOR VASILIEV, New Mexico State University — We apply *ab initio* computational methods based on density functional theory to study the transport properties of p-n junctions made of single-walled carbon nanotubes and graphene nanoribbons. The p-n junctions are formed by doping the opposite ends of carbon nanostructures with boron and nitrogen atoms. Our calculations are carried out using the SIESTA electronic structure code combined with the generalized gradient approximation for the exchange-correlation functional. The transport properties are calculated using a self-consistent nonequilibrium Green's function method implemented in the TranSIESTA package. The modeled nanoscale p-n junctions exhibit linear I-V characteristics in the forward bias and nonlinear I-V characteristics with a negative differential resistance in the reverse bias. The computed transmission spectra and the I-V characteristics of the p-n junctions are compared to the results of other theoretical studies and to the available experimental data.

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