Electronic and transport properties of carbon nanoribbons: edge effects and nitrogen doping

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Graphene is a very promising material for future applications in nanoelectronics and molecular devices. Depending on the termination of its edges, graphene can form zigzag or armchair nanoribbons. The ground state of the zigzag nanoribbons is well known to be spin polarized in calculations, while this has not been observed by experiments. We explain this discrepancy by investigating the electronic properties of different edge structures within density functional theory and show that even a small fraction of defects at the edges suppresses spin polarization.

We also investigate n-type doping of carbon nanoribbons by nitrogen. We find that the doping of nanoribbons is profoundly affected by their 1D structure, the interaction with edge states, and the symmetry of the ribbon. Nitrogen segregation, doping effects on magnetization and impurity-induced carrier scattering will be discussed. For some nanoribbons, impurity scattering results in low n-type conductance, while others are suitable for high-speed devices.