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Edge states and nitrogen substitutional doping in carbon nanoribbons JIE JIANG, NC State U., Raleigh, WENCHANG LU, JERRY BERNHOLC, NC State U., Raleigh; CSMD, ORNL , PIOTR BOGUSLAWSKI, NC State U., Raleigh; IPPAS, Poland — The edge states in carbon nanoribbons and the electronic and magnetic properties in N-doped carbon nanoribbons are investigated within density functional theory. While the ground state of zigzag ribbons is spin polarized, defects at the edges destroy the polarization and lead to a non-magnetic ground state. Scanning tunneling spectroscopy will thus show different features depending on edge quality. Turning to substitutionally doped carbon nanoribbons, the impurity states are elongated along the ribbon width by edge and confinement effects, which also affect their ionization energies in armchair ribbons. Formation energy calculations reveal that N atoms preferentially occupy edge sites in carbon nanoribbons. The extra electron from the donor suppresses the spin-polarization and tailor the relative magnetization at the two edges in zigzag ribbons. The interplay of impurity and edge states in zigzag ribbons leads to rich electronic effects, resulting in semiconducting or metallic behavior depending on the dopant position.

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