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Edge effects on impurity states in carbon nanoribbons JIE JIANG, NC State U., Raleigh, WENCHANG LU, NC State U., Raleigh, CSMD, ORNL, PIOTR BOGUSLAWSKI, IPPAS, Poland, JERRY BERNHOLC, NC State U., Raleigh, CSMD, ORNL — We investigated the electronic structure and spin polarization of nitrogen-doped carbon nanoribbons with DFT. We find enhanced segregation in zigzag nanoribbons, due to interplay between impurity states in the valence bands and the edge states. The magnetization is partially quenched by the doping. We also find that the three armchair nanoribbons (ARs) families 0, 1, 2 as mod (n+1, 3)=0, 1, 2 behave differently in doping. In family 1, the impurity level is in the band gap. Its ionization energy decreases with the increase of ribbon width and it oscillates with the dopant position. The joint effects of high mobility and width-dependent ionization energy make the family 1 AR attractive n- type semiconductors for electronic devices. The impurity level in families 0 and 2 is a resonance in the conduction bands, which strongly influences the transport properties by decreasing the conductivity near the impurity level.

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