

Edge states and defects in carbon nanoribbons

Jie Jiang, Wenchang Lu, Jerry Bernholc

*Department of Physics, NC State University
Raleigh, NC 27695-7518, USA*

The local density of states (LDOS) of edge states in carbon nanoribbons is investigated within density functional theory. The discrepancy in scanning tunneling spectroscopy experiments is explained by the calculated LDOS, which shows different features around the Fermi level in spin-polarized and non-spin-polarized cases. The latter occurs for mixed or defected edges. Turning to nitrogen doping of carbon nanoribbons, our calculations show that the substitutional doping is energetically preferable to pyridine-type doping and that nitrogen atoms prefer to segregate to the edge. The impurity-induced states can mix with edge states either below or above the Fermi level, depending on dopant positions, leading to either a metallic or a semiconducting system. Furthermore, with substitutional dopants near the ribbon edges, magnetism around the dopants is suppressed. Therefore, magnetic properties of nanoribbons can be tailored by doping.