Do Stone-Wales defects alter the magnetic and transport properties of single-walled carbon nanotubes?

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Finite zigzag single-walled carbon nanotubes (SWCNTs) of some nanometers in length and modified by a topological defect of the Stone-Wales type were investigated by density functional theory (DFT) computation. Geometric changes of the regular hexagonal reference structures as well as alterations of their energetic, magnetic, and transport characteristics induced by the presence of the defect were recorded and discussed as a function of the tube length. SWCNT prototypes with hydrogen and fullerene hemisphere termination, and center as well as edge site defects are included in this study. The resulting four basic system types are characterized in terms of the Stone-Wales defect stabilization energy, as well as the energy gaps of the systems with and without Stone-Wales defects. While the magnetism of a zigzag SWCNT reacts sensitively to the nature and number of external adsorbates, it remains unaffected by the presence of Stone-Wales defects. However, the calculated current-voltage characteristic for a representative SWCNT with and without the defect, as well as the associated differential conductivity show a marked response to the defect for voltages exceeding about 1 V.