Interface States in Carbon Nanotube Junctions

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Carbon nanotubes are one of the most promising materials to develop future nanoelectronics. A progress in this field towards real applications depends on the ability to form junctions between different nanotubes. Recently, the controlled synthesis of carbon nanotube intramolecular junctions has been reported. Intermolecular junctions present often interface states, which are commonly regarded as a drawback in device performance, but they may also provide a means of achieving diode behavior at the nanoscale.

We study the nature and origin of interface states in carbon nanotube intramolecular junctions between tubes. Such states appear usually around the Fermi level and are relevant for transport properties of carbon nanotube junctions. We focus on achiral junctions between (n,n) and (2n,0) tubes, which joined by n pairs of pentagon/heptagone topological defects.

Since the early studies of carbon nanotube junctions it was suggested and commonly accepted that interface states are due to topological defects. However, our results show that these states are not caused by the pentagon/heptagon defects but originate from the edge states of zig-zag nanoribbons and zig-zag (2n,0) tubes. We have found that the number of interface states increases with tube diameter following a multiple-of-three rule. By applying the Born-von Karman boundary condition to an interface between armchair- and zigzag-terminated graphene layers, we are able to precisely explain their number and their energies. Our results give a new vision on the nature of interface states and have implications in other systems, such as graphene vacancies or substitutional impurities.