

Low energy description of defects and boundaries for conducting carbon nanotubes

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We introduce lattice models to describe defects and boundary structures for conducting carbon nanotubes at low energies. In this regime the band structure of the tubes can be simplified by keeping only the two conducting bands, providing an effective description in terms of two parallel chains. We show that imperfections such as impurities, structural defects or caps can be easily included into such models, allowing straightforward physical interpretation of their consequences and reducing significantly the complexity of any calculation. The method is quite general and can be used to study a wide range of possible imperfections in carbon nanotubes. We use it to obtain the electron density patterns expected from a scanning tunneling microscopy experiment for half fullerene caps and for two surface distortions on the body of the tube, the Stone-Wales and the single vacancy defect.