

Zippering Mechanism of Carbon Nanotube Fusion

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We propose a new microscopic mechanism to explain the unusually fast fusion process of carbon nanotubes. We identify the detailed pathway for two adjacent (5,5) nanotubes to gradually merge into a (10,10) tube, and characterize the transition states. The propagation of the fused region is energetically favorable and proceeds in a morphology reminiscent of pants via a zipping mechanism, involving only Stone-Wales bond rearrangements with low activation barriers. The zipping mechanism of fusion can be supported by a time series of High-resolution Transmission Electron Microscopy observations.