Designing Carbon-Based Nanotechnology on a Supercomputer

David Tománek

Michigan State University
tomanek@msu.edu ○ http:/www.pa.msu.edu/~tomanek/

The continuous reduction of device sizes, which is rapidly approaching the atomic level, raises particular challenges in terms of component interconnection and fault tolerance. Due to fundamental limitations imposed on observations by the quantum behavior of these systems, predictive computer simulations emerge as a powerful approach to design complex nanostructures and to understand their behavior [1].

I will show how carbon nanotubes, one of the most promising building blocks of Nanotechnology, can be used as mechanically strong, self-repairing interconnects, similar to the VELCRO bond [2]. Combined electronic structure and quantum transport calculations for metal-nanotube junctions reveal that the optimum electrical contact should be neither too strong, nor too weak [3]. In contrast to bulk systems, carbon nanotubes and related nanostructures demonstrate an unexpected defect tolerance, assisted by a self-healing mechanism, which may be initiated by thermal and electronic excitations [4]. In particular, irradiation by monochromatic light emerges as the most efficient way to reconnect atoms or to desorb unwanted impurities [5].

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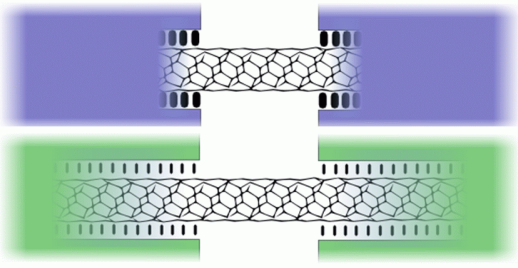
Schematic model of nanoVELCRO



Optimizing the contact between a nanotube and a metal lead