Nanotubes, Buckyballs, and the Nanotechnology Revolution

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].

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 [2]. In contrast to bulk systems, carbon nanotubes and related nanostructures demonstrate an unexpected defect tolerance, assisted by a self-healing capability when thermally and electronically excited [3]. In nanotubes, electronic excitations decay very slowly [4]. Since bonding in the excited state differs significantly from the ground state, photo-chemical reactions [5] and ion beam irradiation [6] emerge as powerful tools to selectively modify nanostructures.

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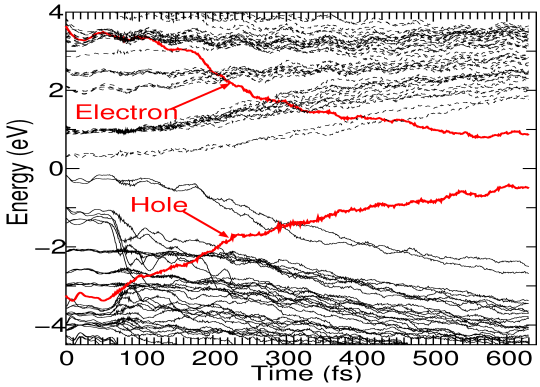
[5] Yoshiyuki Miyamoto, Noboru Jinbo, Hisashi Nakamura, Angel Rubio, and David Tománek, Photodesorption of oxygen from carbon nanotubes, Phys. Rev. B **70**, 233408 (2004).

[6] Arkady V. Krasheninnikov, Yoshiyuki Miyamoto, and David Tománek, Role of electronic excitations in ion collisions with carbon nanostructures, Phys. Rev. Lett. **99**, 016104 (2007).



Time-dependence of Kohn-Sham state following an electron-hole excitation in a (3,3) carbon nanotube [4].

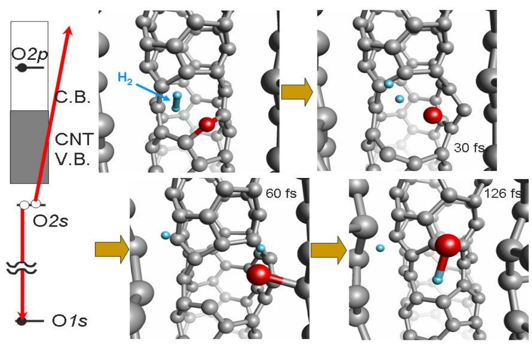


Photo-chemistry in nanotechnology: Selective deoxidation by photoexcitation [5].