

Abstract Submitted
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Changing Carbon Nanostructures by Irradiation¹ DAVID TOMÁNEK, Michigan State University — Changes in the force field of carbon nanostructures immediately following irradiation by light and electrons may cause important structural changes. Exposure to light may modify the morphology at the apex of carbon nanohorns during Raman spectroscopy observations [1], or exfoliate graphite layer-by-layer upon exposure to specifically shaped femtosecond laser pulses [2]. Irradiation by electrons may significantly improve the structural integrity and mechanical properties of low-quality multi-wall carbon nanotubes grown by Chemical Vapor Deposition [3]. *Ab initio* molecular dynamics calculations in the electronic ground and excited state help to analyze the microscopic mechanisms underlying these structural changes including photo-activated Stone-Wales transformations, cross-linking of nanotube walls at extended defect sites, and charge redistribution causing detachment of graphene monolayers.

[1] T. Fujimori *et al.* (in preparation).

[2] Y. Miyamoto *et al.*, Phys. Rev. Lett. **104**, 208302 (2010).

[3] M. Duchamp *et al.*, J. Appl. Phys. **108**, 084314 (2010).

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