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Time-Domain Ab Initio Studies of Phonon-Induced Relaxation of Electronic Excitations in Carbon Nanotubes[1]

OLEG PREZHDO, University of Washington

Electron-phonon interactions in carbon nanotubes (CNT) determine response times of optical switches and logic gates, the extent of heating and energy loss in CNT wires and field-effect transistors, and even a mechanism for CNT superconductivity. Numerous time-resolved experiments have revealed intriguing features of the electron-phonon relaxation in CNTs in response to external stimuli. We report the ab initio studies of the relaxation performed in real-time, directly mimicking the experimental data. The results reveal a number of unexpected features of the relaxation processes, including the differences between the intraband relaxation and electron-hole recombination, the photoexcitation energy dependence of the relaxation, the importance of defects, the dependence on the excitation intensity, and a detailed role of active phonon modes.

[1] B. F. Habenicht, C. F. Craig, O. V. Prezhdo, "Electron and hole relaxation dynamics in a semiconducting carbon nanotube", *Phys. Rev. Lett.* **96** 187401 (2006); *Virtual J. Nanoscale Sci. & Tech,* May 29, 2006; *Virtual J. of Ultrafast Science*, June 2006

[1]In collaboration with Brad Habenicht and Colleen Craig, University of Washington.