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

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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.


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