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Time-Domain Ab Initio Studies of Photoinduced Electron-Phonon Dynamics in Carbon Nanostructures.

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The electron-phonon interactions in carbon nanotubes and nanoribbons determine the response times of optical switches and logic gates, the extent of heating and energy loss in nanowires and field-effect transistors, and even a superconductivity mechanism. We have developed state-of-the-art non-adiabatic molecular dynamics techniques and implemented them within time-dependent density functional theory in order to model the ultrafast photoinduced processes in carbon nanostructures at the atomistic level and in real time. Our ab initio studies directly mimic the experimental data and reveal many intriguing features of the excitation dynamics, including non-radiative fluorescence quenching, fast intrinsic intraband relaxation, phonon-induced component of fluorescence linewidths, the importance of defects, the dependence of the relaxation rates on the excitation energy and intensity, spin-orbit interaction and a detailed understanding of the role of active phonon modes.