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Real-time *ab initio* simulations of excited-state dynamics in nanostructures[1]

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Combining time-dependent *ab initio* density functional calculations for electrons with molecular dynamics simulations for ions, we investigate the effect of excited-state dynamics in nanostructures. In carbon nanotubes, we find electronic excitations to last for a large fraction of a picosecond.[2] The de-excitation process is dominated by coupling to other electronic degrees of freedom during the first few hundred femtoseconds. Later, the de-excitation process becomes dominated by coupling to ionic motion. The onset point and damping rate in that regime change with initial ion velocities, a manifestation of temperature dependent electron-phonon coupling. Considering the fact that the force field in the electronically excited state differs significantly from the ground state, as reflected in the Franck-Condon effect, atomic bonds can easily be broken or restored during the relatively long lifetime of electronic excitations. This effect can be utilized in a "photo-surgery" of nanotubes, causing structural self-healing at vacancy sites[3] or selective de-oxidation processes induced by photo-absorption.[4] Also, electronic excitations are a key ingredient for the understanding of sputtering processes in nanostructures, induced by energetic collisions with ions.[5]

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[2]Yoshiyuki Miyamoto, Angel Rubio, and David Tomanek, Phys. Rev. Lett. **97**, 126104 (2006).
[3]Yoshiyuki Miyamoto, Savas Berber, Mina Yoon, Angel Rubio, and David Tomanek, Chem. Phys. Lett. **392**, 209 (2004).
[4]Yoshiyuki Miyamoto, Noboru Jinbo, Hisashi Nakamura, Angel Rubio, and David Tomanek, Phys. Rev. B **70**, 233408 (2004).
[5]Yoshiyuki Miyamoto, Arkady Krasheninnikov, and David Tomanek (in preparation).