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An ab initio description of cleaning of SWNT with UV light
ABRAM VAN DER GEEST, Colorado School of Mines, KATHRINE HURST, NIST Boulder, MARK T. LUSK, Colorado Scool of Mines — The photodesorption of molecules and its application to the cleaning of single walled carbon nanotubes (SWNTs) has been experimentally demonstrated using a 248 nm laser. The excitation of the carbon nanotube π-plasmon is thought to couple to vibrational modes of the molecule-nanotube bond. An *ab initio* inquiry seeks to validate this hypothesis and optimize the process of nanotube cleaning. The response of SWNTs to an electric field, a description of the enhancement of surface plasmons, and the role of hot electrons are discussed.

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