

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Laser-Shot-Induced Chemical Reactions inside Nanotubes: a TDDFT investigation** HONG ZHANG, Sichuan University, China, YOSHIYUKI MIYAMOTO, NEC, Japan, ANGEL RUBIO, University of the Basque Country, Spain — We present the application of the time-dependent density functional theory (TDDFT) on ultrafast laser pulse which induces dynamics in molecules encapsulated by a nanotube. A strong laser pulse polarized perpendicular to the tube axis induces a giant bond-stretch of an HCl molecule inside both C and BN nanotubes. Depending on the initial orientation of the HCl molecule, the subsequent laser-induced dynamics is different [1]. We also observed a radial motion of the nanotube and vacancies appear on the tube wall when the HCl is perpendicular to tube axis. Furthermore, the disintegration of HCl molecules took place when their molecular axis tilted to tube axis. These simulations are important to analyze light-induced nanochemistry and manipulation of nanostructures encapsulated in organic and inorganic nanotubes. The computational scheme used in present work was a combination of the molecular dynamics and real-time propagation of electron wave functions under presence of strong optical field [2,3]. The energy conservation rule was checked to monitor the numerical stability. [1] Y. Miyamoto, H. Zhang, and A. Rubio, submitted., [2] O. Sugino and Y. Miyamoto, Phys. Rev. B59, 2579 (1999). [3] A. Castro, E. Rasanen, A. Rubio and E. K. U. Gross, Eur. Phys. Lett. 87, 53001 (2009).

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Date submitted: 02 Nov 2010

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