Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Density Functional Calculations of the ^{13}C NMR Chemical Shifts in Single-Walled Carbon Nanotubes JOCHEN AUTSCHBACH, Department of Chemistry, State University of New York at Buffalo, Buffalo, NY 14260-3000, EVA ZUREK, Max Planck Institut für Festkörperforschung, Stuttgart, Germany — Nuclear Magnetic Resonance (NMR) chemical shifts of single–walled carbon nanotubes were computed for capped finite–sized tube fragments and for infinite–length tubes. Molecular density functional calculations using atom–centered basis sets have been performed for the electronic structure and ^{13}C NMR chemical shifts of (5,0), (9,0) and (10,0) single-walled carbon nanotube (SWNT) fragments. For the (9,0) tube, a C_{30}-capped fragment appeared to be a more suitable model to represent an infinite tube then a fragment capped with hydrogens. Thus, the study of the finite (5,0) and (10,0) tubes were restricted to the systems capped with carbon hemispheres. The chemical shift for the (9,0) system [1] is in good agreement with experimental data that were recently obtained from a solution of functionalized nanotubes. Further, we have calculated the ^{13}C chemical shift for a number of infinite small-radius SWNTs using a plane–wave approach. Here, the effect of inter-tube interactions upon the chemical shift was also considered. The results will be compared with those obtained for the finite systems. We believe that our computations may be useful in determining new experimental methods which rely upon NMR to characterize a nanotube sample.
[1] E. Zurek, J. Autschbach, *J. Am. Chem. Soc.* **126**, 13079 (2004).

Jochen Autschbach
Department of Chemistry, State University of New York at Buffalo, Buffalo, NY 14260-3000

Date submitted: 30 Nov 2005 Electronic form version 1.4