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Functional group interactions with single wall carbon NT studied by ab-initio calculations GIANCARLO CICERO, JEFFREY GROSSMAN, ALEKSANDER NOY, GIULIA GALLI, LLNL, Livermore CA — With the goal of designing functionalized nanotube materials, recent AFM measurements have succeeded in determining the force between individual chemical groups an single-wall carbon nanotubes (SWCNT) [1]. In order to rationalize and understand these experimental results, we have performed Density Functional Theory calculations for a number of structural arrangements of model tips functionalized with the same groups as those used experimentally. Our calculations include full geometry optimization of the composite SWCNT/tip system as well as 'pulling-out' simulations to compute interaction forces. We considered (14×0), semi- conducting tubes, and AFM tips where modeled by a SiH_3CH_2-X molecule, with X- representing -CN, -CH_3, -NH_2 or -CH_2OCH_2. As X is varied, computed forces reproduce the same trend as that observed experimentally when n-doped SWCNT are considered; significantly different trends are observed for neutral and p-doped tubes. We propose that the polar solvent present in the experimental setup may be responsible for the n-doping of the nanotube suggested by our calculations. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48. [1] M.C. LeMieux *et al*, preprint

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